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ON THE INFLUENCE OF ELECTRON–ELECTRON CORRELATION ON THE CURRENT–VOLTAGE CHARACTERISTICS OF A SHORT MOLECULAR WIRE

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It is demonstrated that detailed information can be gained on the inelastic mechanism of correlated electron transfer through a molecular wire if one analyses the current behavior in dependence on the strength of the external electric field. The approach is complementary to the derivation of the current–voltage characteristics, and the given analysis of the current-length effect observed at a fixed electric field-strength allows to specify the influence of the blocking transmission factor on incoherent electron transfer. It is found that at small external electric field-strength the current through a regular molecular wire exhibits an Ohmic behaviour while at strong fields electron–electron correlations lead to an exponential decrease of the current.

Keywords: molecular wire; electron transfer; Coulomb repulsion; voltage

1. INTRODUCTION

Today it is expected that a further miniaturization of electronic circuits may be achieved if molecular nanostructures are used. [1–3] Serious progress in molecular electronics is related to research work done in the middle of the nineties. Here it became possible to measure the micro–current a single molecule (cf. e.g.) [4–6]. Meanwhile, various theoretical models of a single–molecule conductivity are proposed to explain current–voltage (I–V) characteristics, in mesoscopic system like the "microelectrode–molecular wire–microelectrode" (M-W-M) system [8–15]. The models are intended to clarify the basic physical effects related to the formation of an elastic as well as an inelastic inter–electrode current. For example, the role of inter–site electronic coupling and the coupling to

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vibrational modes has been discussed. The Coulomb repulsion between different transferring electrons could be characterized, and it became possible to study the control of micro-currents by external fields.

The goal of the present communication is to clarify in more detail a mechanism leading to the formation of an inelastic current through a short molecular wire. This problem has been recently considered in Refs. [16–18] where a kinetic scheme of hopping electron transfer (ET) through the wire has been proposed. Just in short wires (of 25–40 Å length) the Coulomb interaction has been shown to forbid the simultaneous transmission of more than a single excess electron, and just this interaction originates nonlinearities in I–V-characteristics. In the present communication we will concentrate on the current behaviour in dependence on the length of the regular wire. Interestingly, the results becomes more clear if one utilizes the I–ε characteristics instead the I–V one. This is dictated by the fact that if the strength of electric field, ε, is fixed, then the ramp between the neighbouring wire units is conserved independently on the number of units, and thus the length effect becomes more transparent.

2. KINETIC MODEL AND BASIC FORM OF AN INTER–ELECTRODE CURRENT

The mechanism of inter-electrode current formation through a molecular wire depends strongly on the relations between the characteristic times of the dynamic and dissipative processes in the complete M-W-M system. [7–10,16,18–20] If dissipative processes are weak then the wire mediates a pure elastic tunnel current. Fast intra–state relaxation leads to the formation of an inelastic current through the wire. To evaluate an inter-electrode current mediated by a short molecular wire we apply a hopping model proposed in Refs. [16,17] In the respective model the inelastic ET is characterized by single–electron transition rate constants represented in (Fig. 1). The rates $\chi_{L(R)}$ and $\chi_{-L(-R)}$ refer to transitions between the electrodes and the corresponding terminal wire units, while the rates $g_1, g_2, \ldots g_{N-1}$ and $r_2, r_3, \ldots r_N$ specify the transitions of the transferred electron between neighbouring sites of electron localization within the wire. It is assumed that the sites of electron localization, $n = 1, 2, \ldots N$, are separated by the bridging structures B. Besides, the terminal wire units, $n = 1$ and $n = N$, are separated by the spacers B_e. It is very important for the model, that a strong Coulomb repulsion between the transferring electrons inhibits the presence of more than one excess electron in the wire. Therefore, the current is formed by the motion of single electrons with the above mentioned rates while the Coulomb interaction is reflected

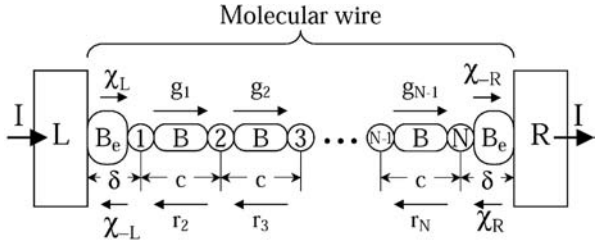

FIGURE 1 Kinetic scheme for the formation of an inter–electrode current through a molecular wire.

in the current $I(t)$ through a specific transmission factor $W_0(t) = \prod_{n=1}^{N}(1 - P_n(t))$ as

$$I(t) = e\left(\chi_L W_o(t) - \chi_{-L} P_1(t) \prod_{n=2}^{N} P_n(t)\right) \tag{1}$$

Here, e is the electron charge and $P_n(t)$ denotes the population of the nth wire unit by the transferred electron. These populations are derived from the solution of a nonlinear set of kinetic equations

$$\dot{\mathbf{P}}(t) = -\hat{\mathbf{A}}\mathbf{B}(t) + \mathbf{C}(t), \tag{2}$$

with $\mathbf{B}(t) \equiv \mathbf{U}(t)W_0(t)$, $\mathbf{C}(t) \equiv \mathbf{C}W_0(t)$. The time-dependent vectors $\mathbf{P}(t)$ and $\mathbf{U}(t)$ are defined by the site populations $P_n(t)$ and auxiliary functions $U_n(t) \equiv P_n(t)/(1 - P_n(t))$, respectively. The components C_n of the vector $\mathbf{C}$ and the elements A_{nm} of the matrix $\hat{\mathbf{A}}$ are defined as

$$C_n = \chi_L \delta_{n,1} + \chi_R \delta_{n,N} \tag{3}$$

and

$$\begin{aligned} A_{nm} = \lfloor (\chi_{-L} + g_1)\delta_{n,1} + (g_n + r_n)\big(1 - \delta_{n,1}\big)\big(1 - \delta_{n,N}\big) + \\ + (\chi_{-R} + r_N)\delta_{n,N}\rfloor \delta_{n,m} - g_{n-1}\big(1 - \delta_{n,1}\big)\delta_{n,m+1} \\ - r_{n+1}\big(1 - \delta_{n,N}\big)\delta_{n,m-1}. \end{aligned} \tag{4}$$

Below we will restrict ourselves to an exclusive consideration of the stationary regime of transfer processes. At stationary conditions the site populations and thus the current become time–independent quantities. The stationary site populations P_n are derived from the set (2) for $\dot{\mathbf{P}}(t) = 0$. For such a condition the set (2) is reduced to a set of linear algebraic equations

$$\sum_{m=1}^{N} A_{nm} U_m = C_n. \tag{5}$$

The stationary current (1) can be represented in the simple form

$$I = eW_0 J, \tag{6}$$

where the quantity

$$J = \frac{1}{\mathrm{Det}(N)}(\chi_L g_1 \ldots g_{N-1}\chi_{-R} - \chi_R r_N \ldots r_3 r_2 \chi_{-L}) \tag{7}$$

appears as a net electron flow (the symbol $\mathrm{Det}(N)$ denotes the determinant of matrix $\hat{\mathbf{A}}$). In Eq. (6), the quantity

$$W_0 = \prod_{n=1}^{N}(1 - P_n) = \prod_{n=1}^{N}(1 + U_n)^{-1} \tag{8}$$

gives the transmission factor. The form of W_0 reflects the validity of a particular exclusive principle in a short wire. If strong Coulomb repulsion takes place between the transferred electrons only a single electron can move through the wire.

Solving the set (5) for a given number of wire units one can derive an analytical expression for both, the transmission factor W_0 and the flow J. For instance, at $N = 4$ one obtains

$$\mathrm{Det}(4) = \chi_{-L}(\chi_{-R} + r_4)\, r_3\, r_2 + \chi_{-R}(\chi_{-L} + g_1)\, g_2 g_3 + \chi_{-L}\chi_{-R}\, r_2\, g_3 \tag{9}$$

with

$$J = \frac{1}{\mathrm{Det}(4)}(\chi_L g_1 g_2 g_3 \chi_{-R} - \chi_R r_4 r_3 r_2 \chi_{-L}). \tag{10}$$

The transmission factor is defined by Eq. (8) where

$$\begin{aligned}
U_1 &= \frac{1}{\mathrm{Det}(4)}\{\chi_L[(\chi_{-R} + r_4)r_3 r_2 + (g_2 + r_2)\chi_{-R} g_3] + \chi_R r_4 r_3 r_2\},\\
U_2 &= \frac{1}{\mathrm{Det}(4)}\{\chi_L(\chi_{-R} + r_4)g_1 r_3 + \chi_R(\chi_{-L} + g_1)r_4 r_3 + \chi_L\chi_{-R} g_1 g_3\},\\
U_3 &= \frac{1}{\mathrm{Det}(4)}\{\chi_R(\chi_{-L} + g_1)g_2 r_4 + \chi_L(\chi_{-R} + r_4)g_1 g_2 + \chi_R\chi_{-L} r_4 r_2\},\\
U_4 &= \frac{1}{\mathrm{Det}(4)}\{\chi_R[(\chi_{-L} + g_1)g_2 g_3 + (g_3 + r_3)\chi_{-L} r_2] + \chi_R g_1 g_2 g_3\}.
\end{aligned} \tag{11}$$

In the case of regular molecular wire and if

$$\alpha \equiv g_1 = g_2 = \ldots = g_{N-1}, \quad \beta = \gamma\alpha \equiv r_2 = r_3 = \ldots = r_N, \tag{12}$$

one can derive a general expression for J and U_n,

$$J = \frac{\xi\chi_L\zeta_L(1-\gamma)[1 - \exp(-eV/k_B T)]}{1 - \gamma^{N-1} + \zeta_L(1 + \xi\gamma^{N-1})(1-\gamma)}, \tag{13}$$

$$U_n = \frac{\chi_L}{\chi_{-L}} \frac{1 - \gamma^{N-n} + \lambda\gamma^{N-n}\left(1 - \gamma^{n-1}\right) + \zeta_L\gamma^{N-n}(1-\gamma)(\xi+\lambda)}{1 - \gamma^{N-1} + \zeta_L(1+\xi\gamma^{N-1})(1-\gamma)} \tag{14}$$

where the ratios of rate constants, $\zeta_L \equiv \alpha/\chi_{-L}$ and $\xi \equiv \chi_{-L}/\chi_{-R}$, are introduced along with the parameters

$$\begin{aligned} \gamma \equiv \beta/\alpha = \exp(-eVc/Lk_BT), \qquad \lambda &\equiv \exp[(\Delta E_L - \Delta E_R)/k_BT] \\ &= \exp(-2\,eV\delta/Lk_BT). \end{aligned} \tag{15}$$

The parameter γ strongly depends on the voltage bias (Vc/L) between neighbouring sites spaced by the distance c, while the parameter λ varies with the factor $(V\delta/L)$ specifying the voltage bias between the terminal unit and the corresponding electrode. A total voltage bias along the wire of length $L = 2\delta + (N-1)c$ is equal to the quantity V.

The general expressions (6)–(8) and their particular analytic form (13)–(15) allow us to evaluate various regimes of stationary ET processes through a molecular wire if one specifies the concrete form of the rate constants.

3. MAIN RESULTS AND DISCUSSION

In the course of hopping processes the transferred electron is captured by the wire units so that each hopping between the nth and n'th unit is characterized by the rate constant $\kappa_{n\to n'}$. In line with the scheme of (Fig. 1) inter-site rate constants are denoted by $g_n \equiv \kappa_{n\to n+1}$ and $r_n \equiv \kappa_{n+1\to n}$, $(n = 1, 2, \ldots, N-1)$. To specify the constants we utilize the Jortner form which reads for a regular wire as [16]

$$\begin{aligned} g_n = \alpha_0\Phi_{\nu_n}, \qquad r_{n+1} &= \exp[-(E_n - E_{n+1})/k_BT]g_n, \\ \Phi_{\nu_n} &= \exp[-S\coth\hbar\omega_0/2\,k_BT]\{[1+n_B(\omega_0)]/n_B(\omega_0)\}^{\nu_n/2} \\ &\quad \times I_{|\nu_n|}\left(2\,S\sqrt{n_B(\omega_0)(1+n_B(\omega_0))}\right). \end{aligned} \tag{16}$$

Here, $n_B(\omega_0) = [\exp(\hbar\omega_0/k_BT) - 1]^{-1}$ is the Bose distribution (ω_0 is the characteristic frequency of the active vibrational mode which strongly couples to a heat bath). Additionally we have $S \equiv \lambda/\hbar\omega_0$ (λ is the reorganization energy), and $I_\nu(z)$ gives the modified Bessel function. The parameter

$$\nu_n \equiv (E_n - E_{n+1})/\hbar\omega_0 \tag{17}$$

defines (in units $\hbar\omega_0$) the energy bias between neighbouring sites of electron localization. The energy of the transferred electron captured by the nth wire unit,

$$E_n = E_0 + eV(1 - x_n/L) + E^{(i)}(x_n), \tag{18}$$

is the sum of the unperturbated energy E_0, the linear ramp, and the polarization shift caused by the electrodes. Following the results of Simmons [21] we approximate this shift by the simple expression

$$E^{(i)}(x_n) = \frac{A}{(x_n/L)(1 - x_n/L)}, \quad (A \approx 5.42/\varepsilon_m L), \tag{19}$$

where the parameter A is given in eV while the position of the nth wire unit, $x_n = \delta + (n-1)c$, and the wire length L are taken in Å. The value of the parameter A varies strongly in dependency on the permittivity of inter–electrode medium ε_m and the wire length.

The polarization shift results in a nonuniform dependence of the energy bias (17) on the applied voltage V even though the wire has a regular structure. We shall show, however, that the presence of such a non-uniformity does not change in principle the $I-V$ and $I-\varepsilon$ characteristics of the wire if compared with those found for an averaged polarization shift. The last supposition provides that the local polarization shift $E^{(i)}(x_n)$ is substituted by an averaged shift $\bar{E}(N)$ so that

$$E_n = E_0 + eV(1 - x_n/L) + \bar{E}(N), \quad \left(\bar{E}(N) = \frac{1}{N}\sum_{n=1}^{N} E^{(i)}(x_n)\right). \tag{20}$$

The electrode–wire, $\chi_{L(R)}$, and wire–electrode, $\chi_{-L(-R)}$, transfer rates can be taken in the form [16]

$$\begin{aligned} \chi_{L(R)} &= \exp\lfloor -\Delta E_{L(R)}/k_B T \rfloor \chi_{-L(-R)}, \\ \chi_{-L(-R)} &= \chi_0 \lfloor 1 - n_F(\Delta E_{L(R)}) \rfloor \Phi_0. \end{aligned} \tag{21}$$

Here, $n_F(\Delta E_{L(R)}) = \left[\exp(\Delta E_{L(R)}/k_B T) + 1\right]^{-1}$ is the Fermi distribution function, and we have $\Delta E_L \equiv E_1 - E_F - eV$, where E_F is the Fermi-energy. The form of the rate constants defined by the Eqs. (16) and (21) (with α_0 and χ_0 representing voltage and temperature independent constants), [18] allow us to analyse both, the temperature dependence and the voltage behaviour of the current at an arbitrary number N of wire units.

Figure 2 displays the nonlinear $I-V$ (and $I-\varepsilon$)- characteristics of a molecular wire. The $I-V$ ($I-\varepsilon$)- behaviour is evaluated in the framework of two models. The first model treats the transferred electron as a probe charge. The corresponding image force potential caused by the electrodes depends strongly on position of the transferred electron within the wire. It brings to different local energy shifts $E^{(i)}(x_n)$, Eq. (19). The second model deals with a simplified approach where the transferred electron experiences an averaged polarization shift so that all local energy shifts, $\bar{E}(N)$, are equal to each other, Eq. (20). One can see from Figure 2 that the simplified model results in a similar nonlinear behaviour of the current in dependence on the applied voltage (or the electric strength). Therefore, to

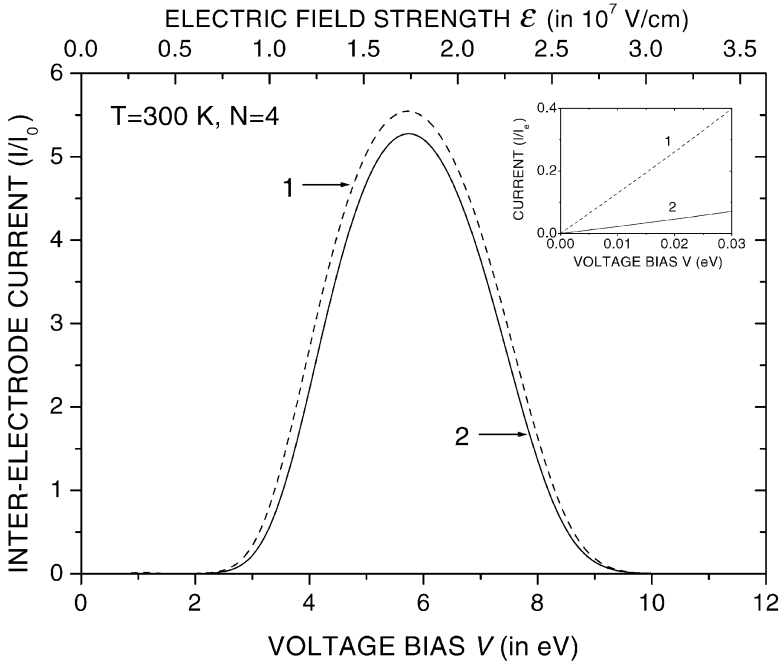

FIGURE 2 Inter–electrode current I, (in units $I_0 = e\chi_0 \cdot 10^{-7}$) *vs*. voltage bias V and electric field strength $\varepsilon = V/L$ at $N = 4$, $L = 33\,\text{Å}$, $\delta = 6\,\text{Å}$, $c = 7\,\text{Å}$, $\varepsilon_m = 3$, $S = 20$, $\omega_0 = 500\,\text{cm}^{-1}$, $\zeta = 10^{-4}$, $\Delta E_0 = 0.5\,\text{eV}$. The inset demonstrates that Ohmic behaviour is only valid at small voltages (in units $I_e \equiv I_0 \cdot 10^{-6}$). Curves 1 and 2 relate to the averaged polarization shift model and the probe charge model, correspondingly.

evaluate the length behaviour of the current one can utilize this simplified description where the local energies of the transferred electron are given by Eq. (20). In this model, the inter–site energy bias (17) becomes independent on the position of the extra electron within the wire, and thus one can employ the analytic expressions (12)–(15).

First we focus our attention to the Ohmic $I-V$ -characteristics which occurs at a small voltage bias (cf. the insertion in Fig. 2). A simplified model yields

$$I \cong eJ = GV, \quad G = G_0 \frac{\zeta \exp(-\Delta E_L/k_B T)}{2\zeta + N - 1}, \tag{22}$$

where $G_0 \equiv e^2\chi_0\Phi_0/k_B T$ is the length independent factor. To derive expression (22) we have used the fact that at a small voltage bias under consideration the inter–site rate constant reads as $\alpha \approx \alpha_0\Phi_0$ and thus

$\zeta_L \approx \zeta \equiv \alpha_0/\chi_0$. The length dependence is located in the factors $2\zeta + N - 1$ and $\exp(-\Delta E_L/k_B T)$. If the limiting step of the ET process is associated with an electron hopping along the wire, then ζ is very small and thus the denominator $2\zeta + N - 1$ reduces to $N - 1$. It means that at a small voltage V the current exhibits the Ohmic behaviour, $I \sim (N-1)^{-1}$ only if the energy gap δE_L depends weakly on the number of wire units. This may appear for the case of a long molecular wire. When the wire is short, a notable distinction from the law $I \sim (N-1)^{-1}$ appears. Figure 3 illustrates the length effect for a small and fixed V. Both, the probe charge model (curve 1) and the averaged polarization shift model (curve 2) results in strong deviations from the Ohmic behaviour (curve 3). [Curve 3 corresponds the model where the averaged polarization shift $\bar{E}(N)$ is taken as a N – independent factor.]

At a large voltage bias, the nonlinearity of the interelectrode current is generally caused by electron–electron correlations (via the transmission factor W_0). This effect has been already discussed in Refs. [16–18] For the length effect under consideration we note that the wire length L may be present in different quantities, in particular, in the site energies (18) (or (20)) as well as in the parameters (15) and (17). To clarify the

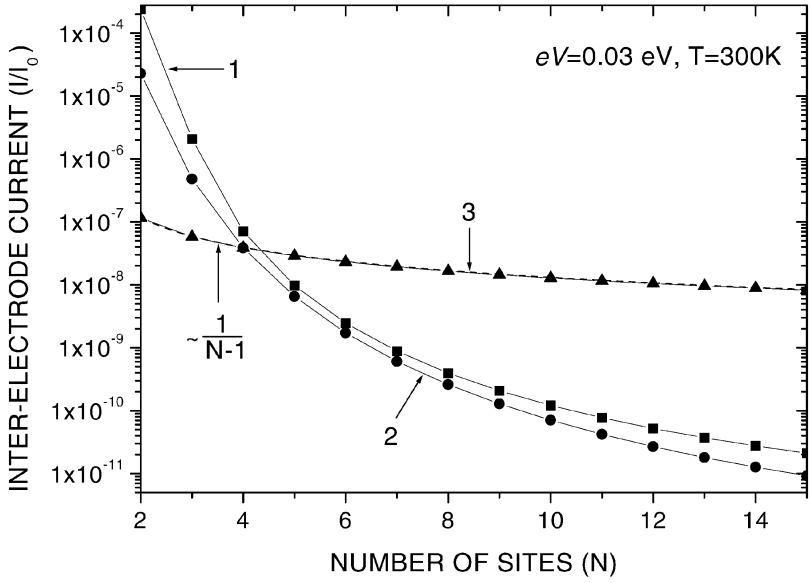

FIGURE 3 Inter–electrode current I (in units I_0) *vs*. the wire units N at small voltage bias V. Curves 1 and 2 correspond to the averaged polarization shift model and the probe charge model, correspondingly. Curve 3 reflects the Ohmic behaviour of the current. (Calculations are done with the parameters of Figure 2.)

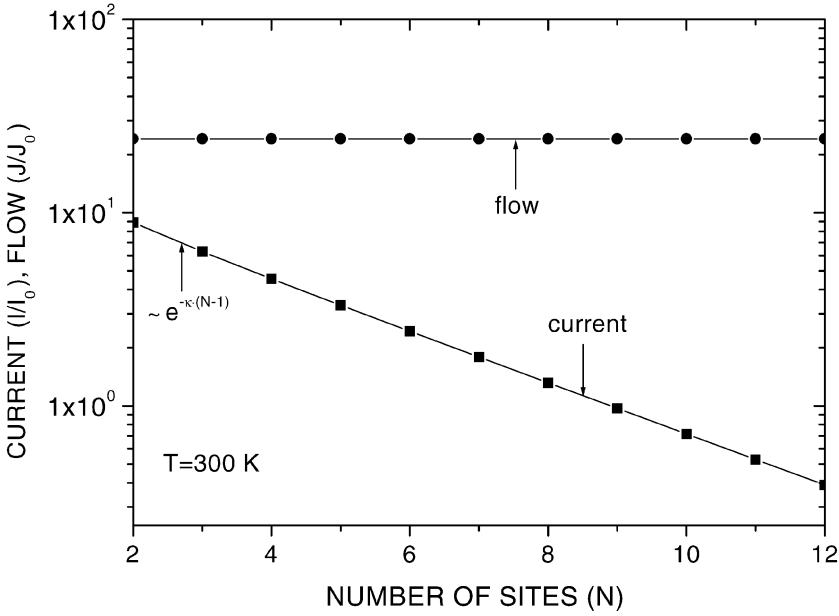

FIGURE 4 Flow J (in units $J_0 = \chi_0 \cdot 10^{-7}$) and inter–electrode current I (in units I_0) *vs*. the wire units N at a strong electric field-strength ε. Calculations have been done in using the averaged polarization shift model and in taking the parameters of Figure 2.

length-problem we consider the formation of a current through a regular wire when a fixed electric field $\varepsilon = V/L$ is applied. In this case, the addition of further wire units does not alternate the ramp and thus the parameters (15) become length–independent quantities. Besides, if one utilizes the averaged polarization shift model then an inter–site energy bias (17) is identical for any pair of sites. This circumstance indicates that the inter–site rate constants (12) are length–independent quantities as well, and thus the $I - N$ behaviour is thought to be given by a rather simple form. Figure 4 demonstrates such a behaviour for large ε. The current decrease is well approximated by an exponential dependence on N. This effect can be explained by strong electron–electron correlation (caused by the Coulomb repulsion) which is accounted for by the transmission factor W_0. Actually, at strong ε the backward processes give a minor contribution in the kinetics of the ET. Therefore, with taking $\gamma \approx 0$ and $\lambda \approx 0$ in Eqs. (13) and (14) we derive

$$J \approx \frac{\chi_L \zeta_L}{1 + \zeta_L}, \quad U_n \approx \frac{\chi_L}{\chi_{-L}} \frac{1 + [\lambda(1 + \zeta_L) + \xi\zeta_L - 1]\delta_{n,N}}{1 + \zeta_L}. \tag{23}$$

At strong ε the quantity ζ_L becomes very large, $\zeta_L \gg 1$. This means that a limiting step of the current formation is the temperature dependent delivery of the transferred electron from the left electrode to the terminal wire unit. In this case, the flow $J \approx \chi_L$ is independent on the number of wire units N. For the same conditions, one may derive $U_1 = U_2 = \cdots = U_{N-1} \approx \chi_L/\alpha$, $U_N \approx \chi_L/\chi_{-R}$ so that $W_0 \approx (1 + \chi_L/\chi_{-R})^{-1}$ $(1 + \chi_L/\alpha)^{-(N-1)}$. A comparison with the general expression (6) allows us to state that for the case where a strong electric field has been applied to the electrodes the current drop (with the increase of the wire length) is completely defined by the blocking transmission factor $W_0 \sim \exp[-\kappa(N-1)]$, $(\kappa \equiv \ln(1 + \chi_L/\alpha))$. Just this result underlines the important influence of electron–electron correlations on the ET in short molecular wires.

REFERENCES

[1] Ratner, M. A., & Jortner, J. (Eds). (1997). Molecular electronics. Oxford: Blackwell Science.

[2] Aviram, A., & Ratner, M. A. (Eds). (1998). Molecular electronics: Science and Technology. Ann. NY. Acad. Sci. Vol. 852. New York: New York Academy of Sciences.

[3] Reed, M. (1999). Molecular–scale electronics. *Proc IEEE*, *87*, 652–658.

[4] Datta, S., Tian, W., Hong, S., Reifenberger, R., Henderson, J. I., & Kubiak, C. P. (1997). Current–voltage characteristics of self–assembled monolayers by scanning tunnelling microscopy. *Phys Rev Lett.*, *13*, 2530–2533.

[5] Seminario, J. M., Zacarias, A. G., & Tour, J. M. (1999). Molecular current–voltage characteristics. *J. Am. Chem. Soc.*, *103*, 7883–7887.

[6] Chen, J., Reed, M. A., Rawlett, A. M., & Tour, J. M. (1999). Large on–off ratios and negative differential resistance in a molecular electronic device. *Science*, *286*, 1550–1552.

[7] Mujica, V., Kemp, M., & Ratner, M. A. (1994). Electron conduction in molecular wires. I. A scattering formalism. *J. Chem. Phys.*, *101*, 6849–6855.

[8] Petrov, E. G., Tolokh, I. S., Demidenko, A. A., & Gorbach, V. V. (1995). Electron–transfer properties of quantum molecular wires. *Chem. Phys.*, *193*, 237–253.

[9] Magoga, M., & Joachim, C. (1997). Conductance and transparency of long molecular wires. *Phys. Rev. B.*, *56*, 4722–4729.

[10] Tian, W., Datta, S., Hong, S., Reifenberger, R., Henderson, J. I., & Kubiak, C. P. (1998). Conductance spectra of molecular wires. *J. Chem. Phys.*, *109*, 2874–2882.

[11] Yaliraki, S. N., Roitberg, A. E., Gonzales, C., Mujica, V., & Ratner, M. A. (1999). The injection energy at molecule/metal interfaces: implication for conductance of molecular junctions from an ab initio molecular description. *J. Chem. Phys.*, *111*, 6997–7002.

[12] Mujica, V., Nitzan, A., Mao, Y., Davis, W., Kemp, M., Roitberg, A., & Ratner, M. (1999). Electron transfer in molecules and molecular wires: geometry dependence, coherent transfer, and control. In J. Jortner & M. Bixon, (Eds.), *Advances in Chemical Physics Series*, Vol.107 (pp. 403–429), series eds. Prigogine I, Rice SA. New York: John Wiley and Sons, Inc.

[13] Mujica, V., Roitberg, A. E., & Ratner, M. (2000). Molecular wire conductance: electrostatic potential spatial profile. *J. Chem. Phys.*, *112*, 6834–6839.

[14] Seminario, J. M., Zacarias, A. G., & Tour, J. M. (2000). Theoretical study of a molecular resonant tunnelling diode. *J. Am. Chem. Soc.*, *122*, 3015–3020.
[15] Nitzan, A. (2001). Electron transmission through molecules and molecular interfaces. *Annu. Rev. Phys. Chem.*, *52*, 681–750.
[16] Petrov, E. G., & Hänggi, P. (2001). Nonlinear electron current through a short molecular wire. *Phys. Rev. Lett.*, *86*, 2862–2865.
[17] Petrov, E. G., Zelinskii, Ya. R., & Hänggi, P. (2001). Nonlinear properties of an inter–electrode current through a short molecular wire. *Mol. Cryst. Liq. Cryst.*, *361*, 209–216.
[18] Petrov, E. G., May, V., & Hänggi, P. (2002). Controlling electron transfer processes through short molecular wires. *Chem. Phys.*, (accepted).
[19] Petrov, E. G., Tolokh, I. S., & May, V. (1997). Magnetic field control of electron motion in molecular nanostructures: steplike behaviour and spin polarization of a bridge–assisted interelectrode current. *Phys. Rev. Lett.*, *79*, 4006–4009.
[20] Petrov, E. G., Tolokh, I. S., & May, V. (1998). The magnetic field influence on the inelastic electron tunnel current mediated by a molecular wire. *J. Chem. Phys.*, *109*, 9561–9573.
[21] Simmons, J. G. (1963). Generalized formula for the electric tunnel effect between similar electrodes separated by a thin insulating film. *J. Appl. Phys.*, *34*, 1793–1802.