One-Dimensional and Quasi-One-Dimensional Models of Quantum Waveguides in an External Field

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The modeling of electron coherent transport in low dimensional systems in an external field has been considered. For quasi-one dimensional systems with a profile defined via plane curve the effect of the influence of a transverse electric field on the transmission coefficient of the system is investigated. The possibility of efficient governing of the transmission of the system via external electric field and qualitative agreement of the simulation results for 1D and 2D models is demonstrated.

1. Introduction

Development and miniaturization in the field of electronic components has achieved the stage, when devices make use of quantum coherent effects. There are two actual development directions, namely, the design of new nanoscale digital electronics components and the development of new media and systems, that deal with quantum behavior in mesoscopic scale

Materials with anomalously high Fermi surface anisotropy are commonly refereed to as one-dimensional systems. Their properties are described in terms of one or two dimensional zone structure, while the rest dimensions are spatially localized. It's evident, that transport characteristics of these systems are highly anisotropic, so while conductivity in chosen directions has typical metallic behavior, in localized dimensions we deal with jumps between layers, or even transport is denied [1]

Despite that one-dimensional model systems were used widely in the beginning of condensed matter physics development, they were abandoned for a long while. These models possessed several anomalous properties (e. g. [1–3]). We emphasize the fact of full wavefunction localization in case of small disorder among mentioned properties.

Interest to one-dimensional systems raised again when research on such substances as $TTF-TCNQ$ (tetrathiafulvalenetetracyanoquinodimethane) ,$(SN)_x$, $(CH)_x$ revealed that their electric properties sufficiently differ from known 3D systems. [4]

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Experiments show that temperature dependence of these such materials conductivity has rather high maximum of $10^5 - -10^6 \Omega^{-1} m^{-1}$ for $TTF - TCNQ$. Also, there is a metal-insulator transition in the range of low temperatures. Moreover, a charge density wave (CDW) mechanism of charge transport was observed in experiments with such systems [2]

Several approaches were introduced to describe electric and transport properties of one and quasi-one dimensional systems [5–11]. They describe frequency and temperature dependence of conductivity, anomalous conductivity fluctuations of mesoscopic samples, effects connected with disorder, quantum localization and some other issues It's also important to investigate an influence of geometry limitations on system quantum properties Several results were obtained for one-dimensional chain of non-trivial shape (waveguide-like system) [12]–[20]. It was shown that bonded states exist in quantum waveguides, and localization is possible in ensembles of these systems. [21].

Consideration of these systems in external fields and in scales where ballistic coherent transport plays important role requires more precise accounting of system geometry and overall model generalization. Analytical description of quantum transport on disordered wires in external electric field is discussed in [21]. Landauer approach is used there along with first approximation of controlling field with perturbation theory.

In this paper we give numerical analysis of controlling electric field effect on one-dimensional chain represented with a curve. Also, we will consider the same system represented with narrow plain waveguide of finite length and the same shape as the above mentioned curve.

2. Localization effects in quasi-one-dimensional systems in external fields

We consider a one-dimensional chain of N scatterers (atoms) located along a curve $z(x) = \exp(-\beta x^2)$ on a plane XOZ exposed to external uniform electric field of intensity $\vec{E}_z$ illustrated on fig.1 Potential energy of an electron $u(x)$ in the point (x, z) equals $E_z z(x)$. In case of small β values the system can be considered as a linear chain $z = 0$ with additional potential. An accelerating potential $E_x L$ is applied to fixed edges of a chain, where E_x is electric field intensity and L is chain length.

We will follow [22], where Krönig-Penney model with disorder is used to calculate conductivity. On the lines of [22]–[23], we put down Krönig-Penney quantum model as follows

$$\left(-\frac{d^2}{dx^2} + \sum_{n=1}^{N} V_n \delta(x - na) + eE_z z(x) + eE_x x \right) \Psi(x) = E\Psi(x) \tag{1}$$

where E – Hamiltonian eigenvalues in units $\hbar^2/2m$, $\hbar$ – Planck constant, m – electron mass, e – electron charge, a – grid parameter, V_n – mean value of scattering atom random potential. Amplitude distribution is uniform

FIG. 1. Stochastic model of one-dimensional system in external field with fixed edges.

Then, as in [22]-[23], time-independent Schrödinger equation can be represented as Poincare map due to the properties of scattering potentials

$$\Psi_{n+1} = \left(\cos k_{n+1} + \frac{k_n \sin k_{n+1}}{k_{n+1} \sin k_n} \cos k_n + V_n \frac{\sin k_{n+1}}{k_{n+1}} \right) \Psi_n - \frac{k_n \sin k_{n+1}}{k_{n+1} \sin k_n} \Psi_{n-1} \tag{2}$$

where $k_n = (E + naE_z + z(na))^{1/2}$, N – number of atoms in chain.

System transparency is as follows [22]

$$t = \frac{k_0}{k_L} \frac{|\exp(2ik_L) - 1|^2}{|\Psi_{N+2} - \Psi_{N+3} \exp(-ik_L)|^2} \tag{3}$$

where $k_0 = \sqrt{E}$, $k_L = \sqrt{E + E_z L}$ and $L = N + 2$.

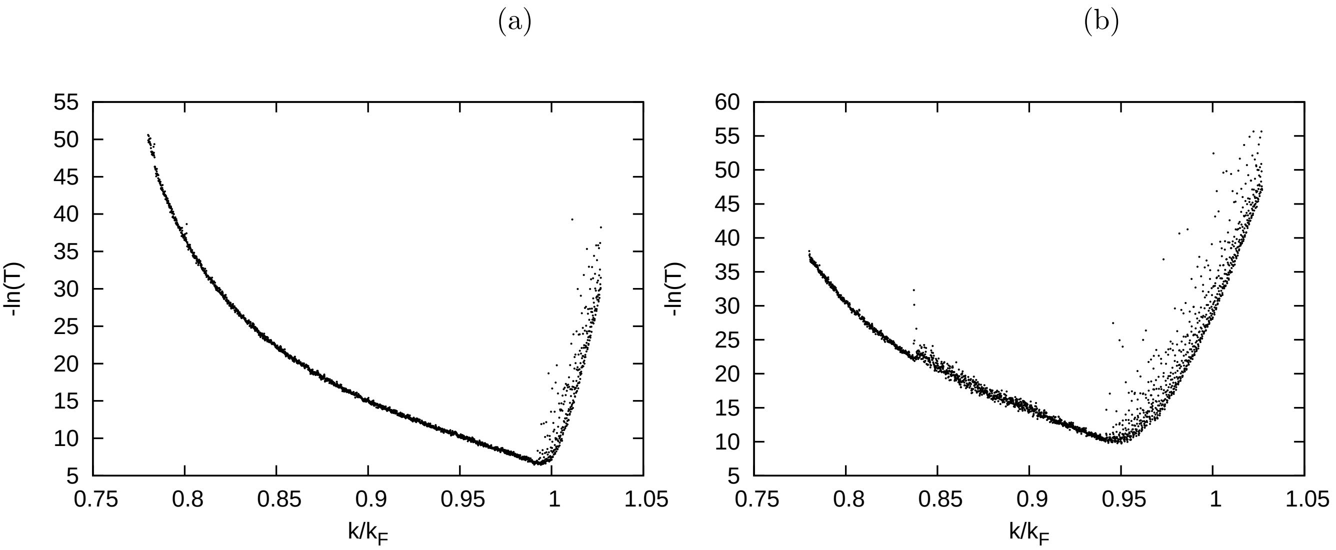

FIG. 2. One-dimensional system transparency $\ln T$ vs. wavenumber k dependence: (a) U_z transverse field maximum value 0.01 eV, (b) U_z maximum value 0.07 eV. k_F stands for Fermi wavenumber.

It is known [9] that a distinguishing feature of one-dimensional models is abnormal conductivity fluctuation. In our system, dispersion is around 2 dB when simulation is held 10000 times for each wavenumber That's why we used a geometric mean of 100000 realizations for each point.

The model reads, that controlling parameter is not the transverse field intensity E_z, but maximal potential energy $U_z = E_z z(0)$ in the electric field System transparency in logarithmic scale vs. electron wavenumber for several U_z values is shown on fig.2. One can find that transverse field makes a sufficient influence on conductivity in the range of wavenumbers close to Fermi vector k_F Thus, it can be stated that transverse electric field can be used to control 1D–system conductivity.

The issue of dependence of transparency on field intensity also makes an interest. As it was mentioned, perturbation theory gives square dependence [24]. Numerical simulation results for T versus U_z are given on fig. 3 Despite theoretical results, there is exponential transparency decrease with the U_z increase.

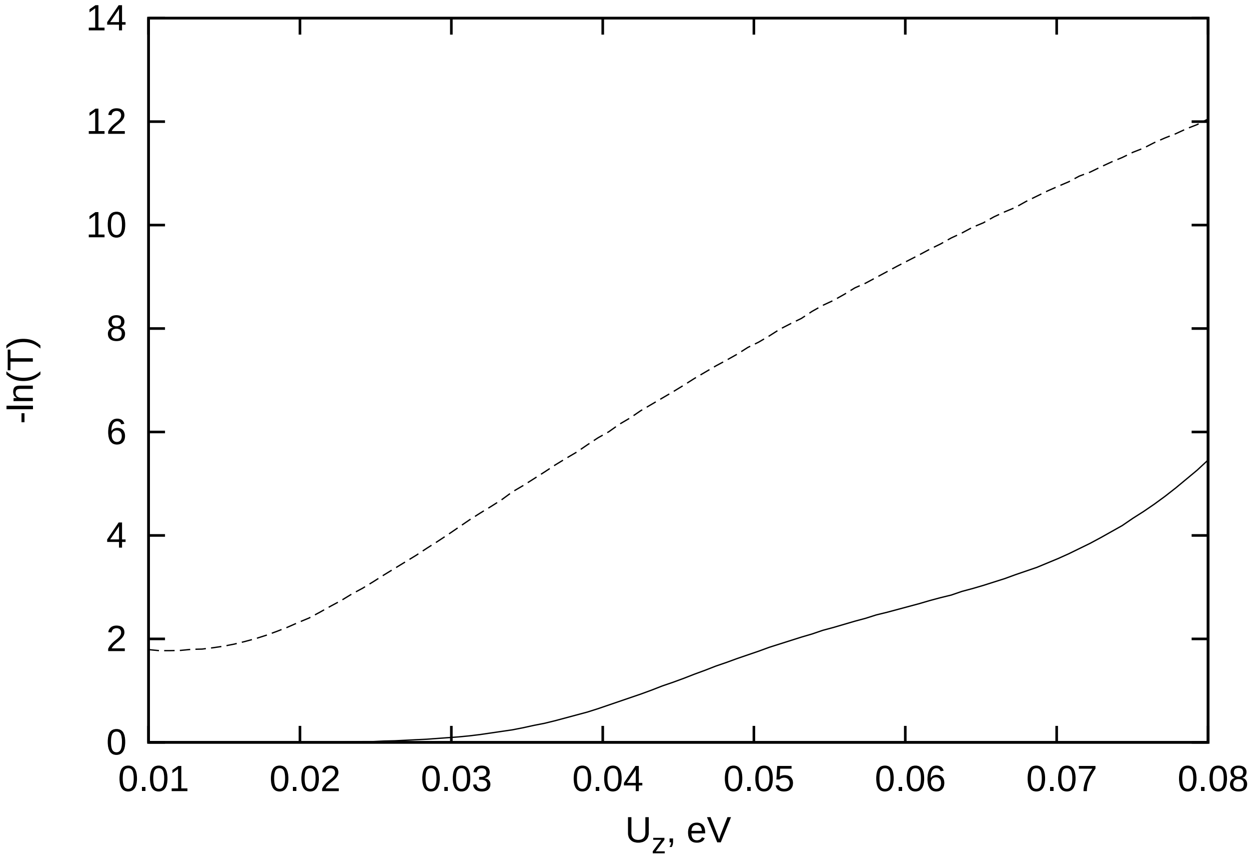

FIG. 3. One-dimensional system transparency logarithm $-\ln T$ versus U_z for wavenumber $k = 0.99\ k_F$: solid line for $N = 100$ atoms, dashed line – $N = 500$ atoms

It should by stated that pure quantum transport mode in scatterers system is considered (localization effects in coherent transport are considerable). Obviously, this fact can be a reason for transparency versus longitudinal field energy dependence observed on fig.4 One can see that the dependence is sufficiently nonlinear, almost exponential This is due to the absence of non-coherent scattering in the system. Such mode is presumed to be achieved in nanoelectronic components within near future.

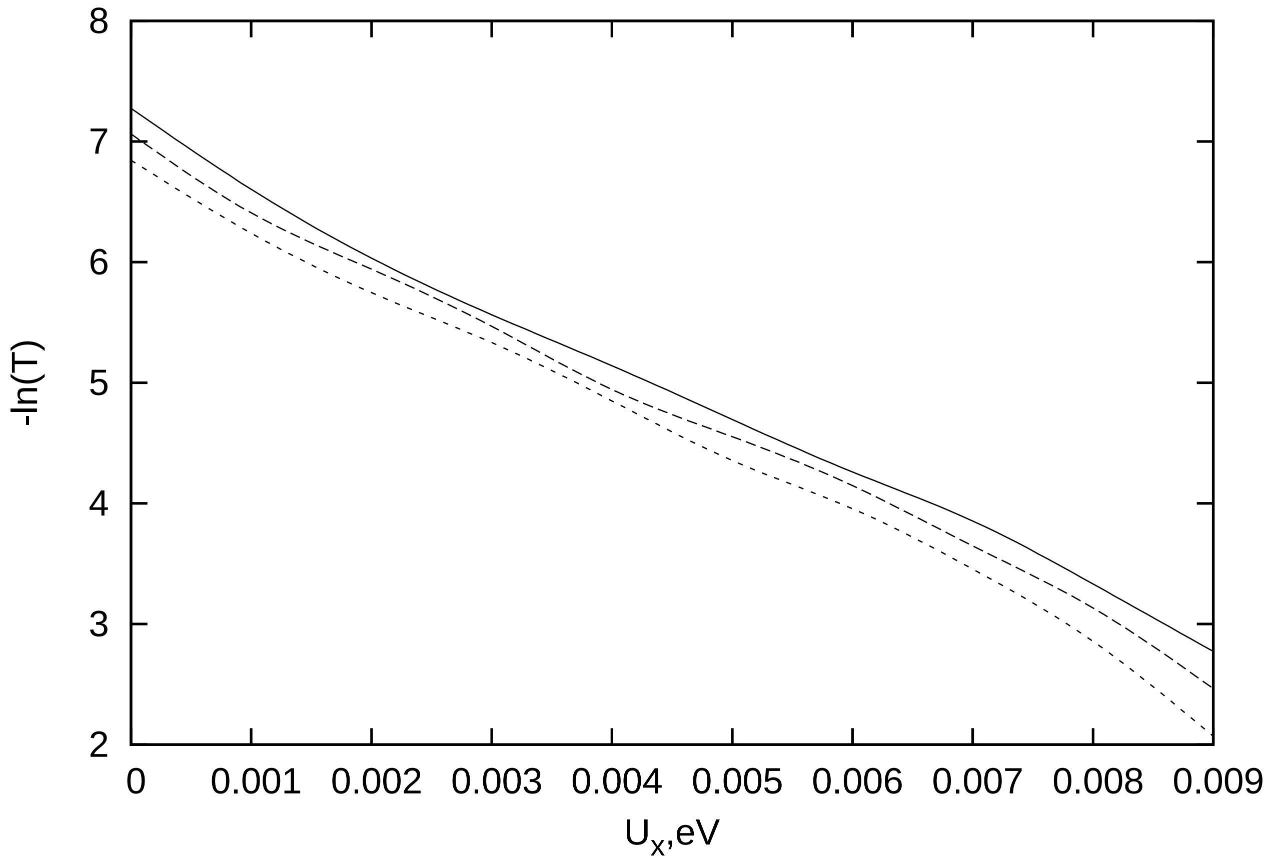

FIG. 4. One-dimensional system transparency $\ln T$ versus U_x dependence for wavenumber $k = 0.99\ k_F$ and several U_z: solid line for $U_z = 0$, dashed line for $U_z = 0.02$ eV, dotted line for $U_z = 0.04$ eV.

To sum up, we can draw a conclusion, that one-dimensional disordered quantum coherent scatterers chain of a nontrivial shape in electric field can possess localization (delocalisation) properties. The dependence of transparency versus field intensity can render a possible use in high-frequency switches for considered systems. However the considered system is rather simplified. That's why we also consider a a plain channel of finite width

3. Field control of conductivity in a curved nanoscale channel

The model represents a nanoscale curved channel (quantum waveguide) of a finite width and shape defined as in previous section with one electron passing through A chain of scatterring atoms of can be allocated inside the channel, and localization phenomena will be caused in that case by both external field and system geometry. Scatterers were simulated via a chain of two-dimensional Gaussian-shaped potentials $u(r) = \exp(-r^2/(2\sigma^2))$ of defined halfwidth $\sigma = 0.1$ nm.

Among approaches to simulation of nanoscale quantum system they usually mark out solution of time-independent Schrödinger equation followed by construction of appropriate transfer-matrix. This approach has considerable disadvantages, namely the requirement to compute a huge number of eigenvalues and eigenfunctions (in our case Hamiltonian ones), and the need of adequate definition of source and drain areas and appropriate border conditions. Another approach is to solve time-dependent Schrödinger equation for a wave packet passing through a defined area. While the number of dimensions is increased by one, two advantageous possibilities appear: a possibility to make an effective parallel supercomputer realization and a possibility to use numerical methods (so-called symplectic integrators) that conserve wavefunction norm. The latter also allows exact charge conservation. We used Split-Step Fourier method [25], a simplectic integrator of error $O(dt^3)$ on a step. Supercomputer implementation is described in [26, 27].

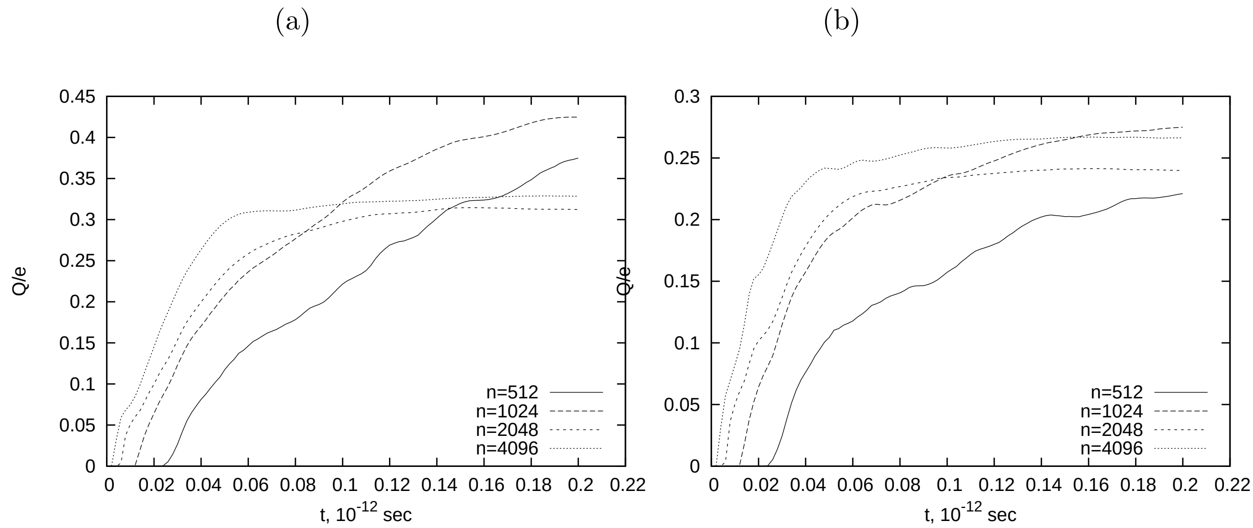

FIG. 5. drain area accumulated charge time dependence for (a) system without scatterring chain (b) with chain.

We were investigating possibility of coherent quantum transport field control, so it was enough to choose an area sufficient for qualitative analysis of corresponding effects. A 30 nm square was chosen. Inside this area there is a curved channel with infinite walls on each side of 2.6 nm flat span. Channel shape is defined as $z(x) = a\exp(-\beta x^2)$, channel length is 20 nm.

Initial wavepacket is a Gaussian-shaped packet in source area with defined speed along the channel. Source and drain areas were supported via accumulating of wavefunction absolute value sqaure in these areas, followed by zeroing these areas on each time step. Thus we obtain charge accumulated in this areas. Asymptotic value of charge accumulated in drain area gives transparency.

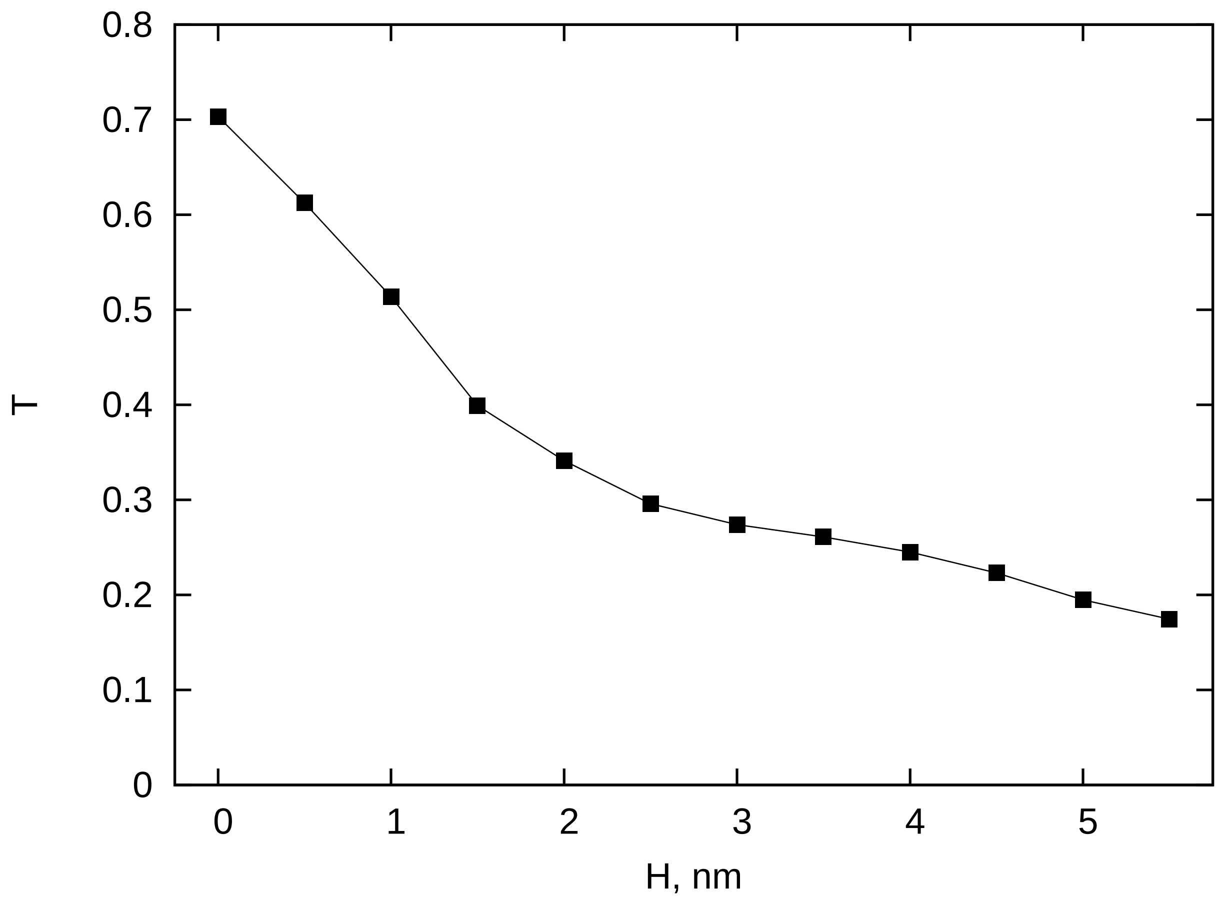

FIG. 6. Transparency T versus profile height H dependency

Numeric analysis reveal that it is enough to use 0.015 nm spatial grid step. Time-dependencies of accumulated charge for several grid resolutions are represented on fig. 5. 2048x2048 resolution gives asymptotic charge value, that differs result obtained for doubled resolution by no more than 10%.

Now let us consider system geometry influence on it's transparency. Curved/straight channel transparency ratio $\frac{T}{T_0}$ vs. bond height dependence is in fig. 6. Curveness-connected phenomena exist, but are relatively small.

A channel of height of 2.4 nm was chosen to evaluate the influence of scattering chain on system transparency. In fig. 7 there are transparency vs. transverse field energy dependencies

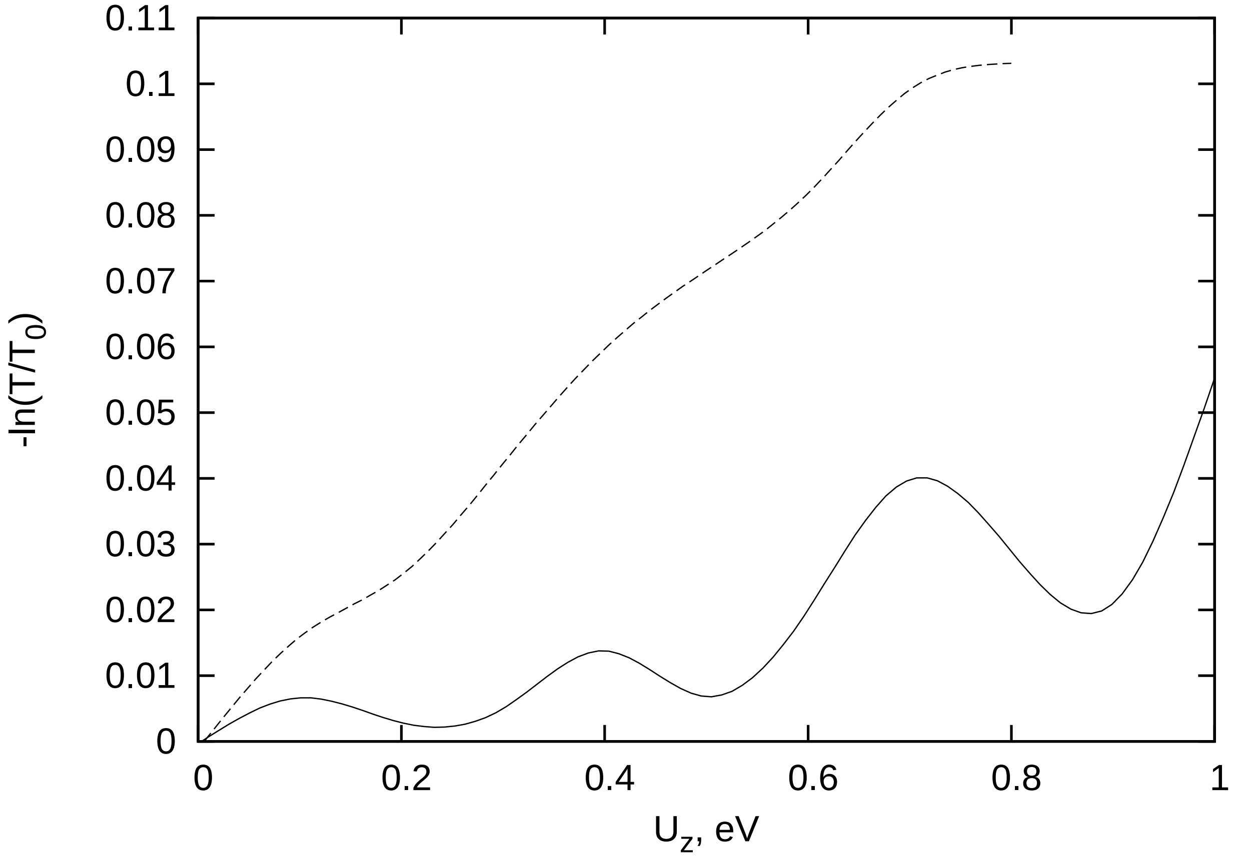

FIG. 7. Transparency $\ln T$ vs. transverse electric field energy dependence. Solid line for system with scatterring chain, dashed line for system without it.

for channels with and without scattering chain. Empty channel transparency is lower than transparency of a channel with scattering chain.

Transparency dependence on transverse field energy for three different longitudinal field energy values is given in 8. Transparency field control works in all this cases.

We use above mentioned $\frac{T}{T_0}$ rate to compare one-dimensional and quasi-one-dimensional models. In fig.9 one can see transparency vs. field energy dependencies for both models. Models are qualitatively compliant.

Conclusion

In the paper we have demonstrated the existence of canal transparency field control in one-dimensional and quasi-one-dimensional systems . Fields of relatively small intensities can be used to control conductivity of these systems in coherent quantum transport mode. Localization

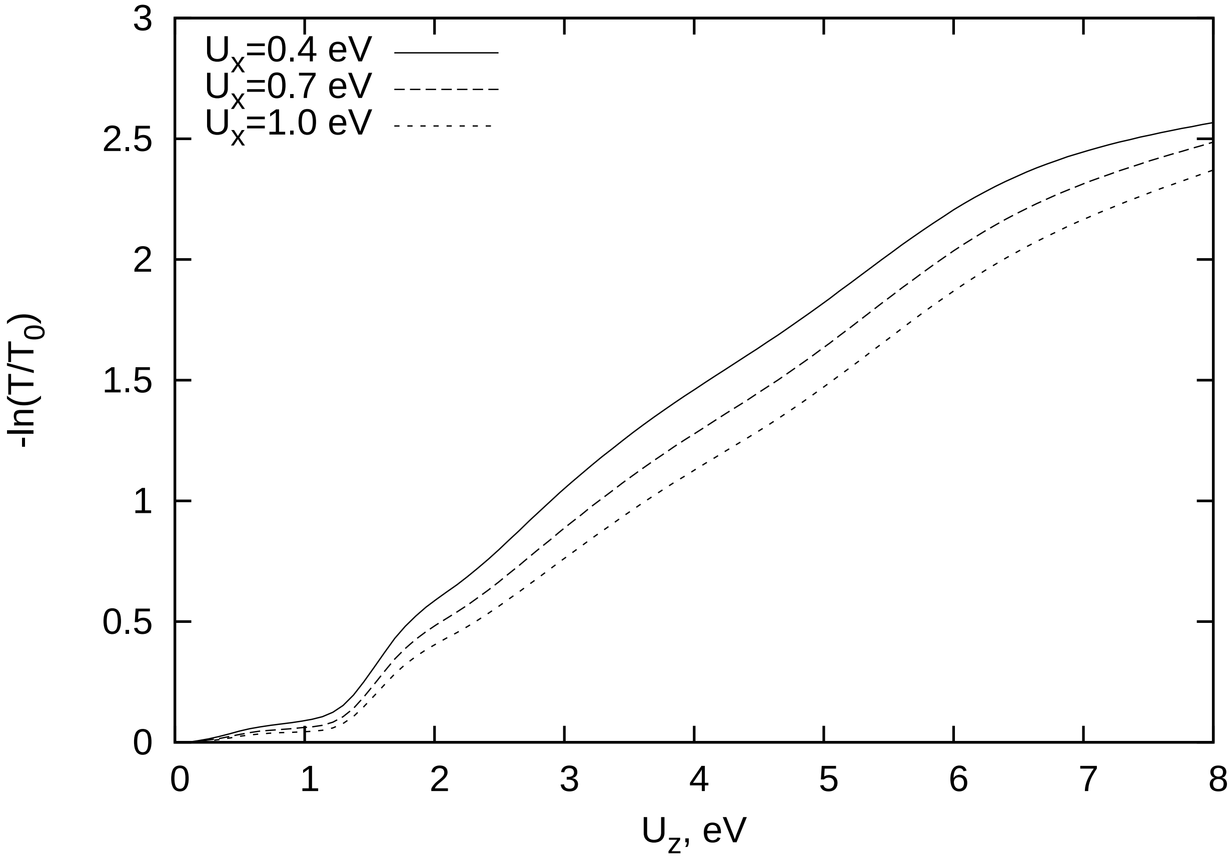

FIG. 8. Curved channel transparency $\ln T$ vs. transverse field energy U_z.

phenomena become exponentially sensitive to the field magnitude. Both considered models have given qualitatively compliant results.

References

[1] S. Kagoshima *et al. One-dimensional conductors.* (Springer-Verlag, 1988).

[2] R. E. Peierls *Quantum theory of solids.* (Oxford, 1955).

[3] V. P. Berezinski JETP. V. 65. P. 1251 (1973).

[4] *Polymers, liquid crystals and low-dimensional solids.* Eds. N. March, M. Tosi. (Plenum Press, 1984).

[5] S.F. Edwards, P.W. Anderson. J. Phys. Vol. F5. P. 965(1975)

[6] A.A. Gogolin. JETP. V. 69. P. 327 (1975).

[7] A.A. Godolin. Phys. Rep. Vol. 86, no. 1. P. 3–53 (1982).

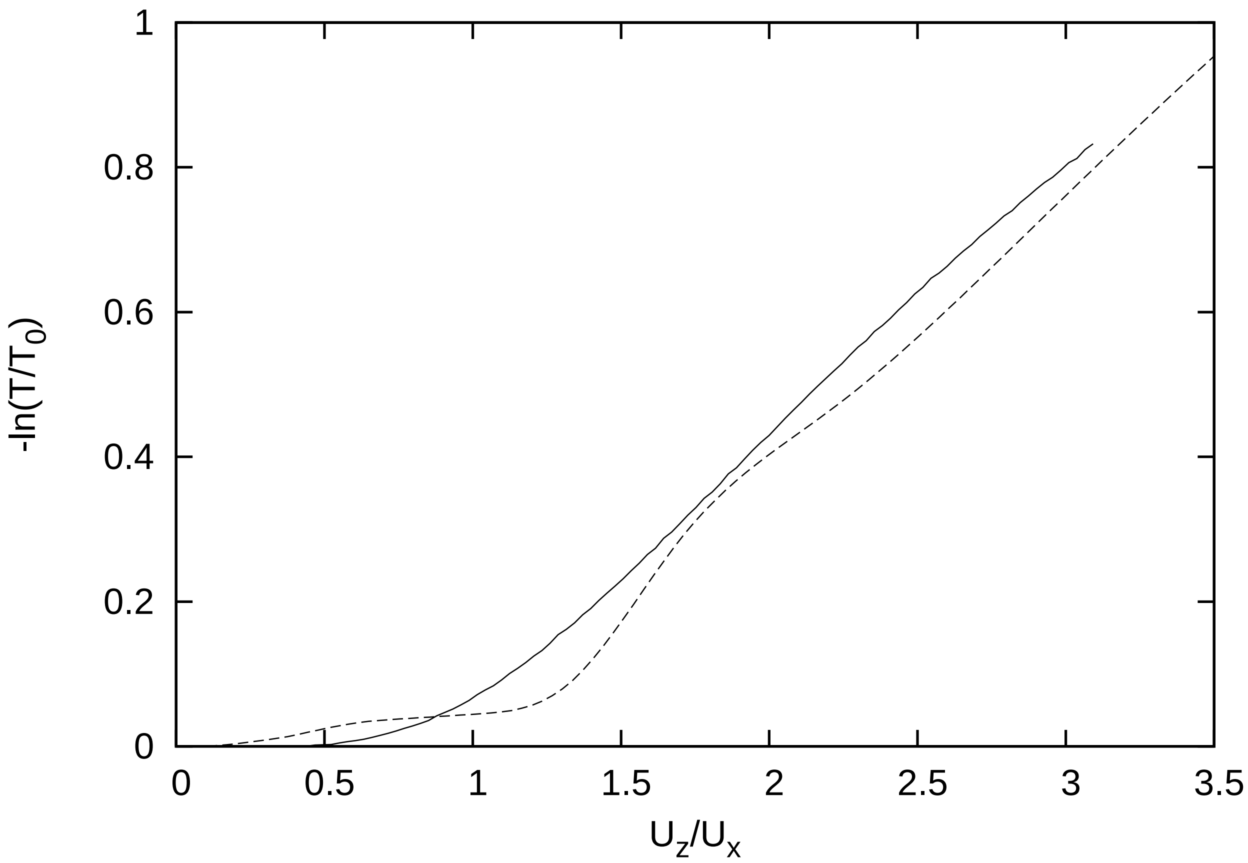

FIG. 9. One-dimensional (solid line) and quasi-one-dimensional (dashed line) models compared

[8] B. Halperin. Phys. Rev. Vol. A139. P. 104 (1965).

[9] B. Shapiro. Phys. Rev. Vol. B34, no. 6. P. 4394–4397 (1986).

[10] A. M. Satalin. JETP. V. 100, 3. P. 1077–1078 (1991).

[11] A.A. Gogolin. Phys. Rep. Vol. 166, no.5. P. 269–351 (1988).

[12] P. Extner and P. Seba. J. Math. Phys. **30**, 2574–2580 (1989).

[13] J. Goldstone and R.L. Jaffe. Phys. Rev. **B45**, 1400–1407 (1992)

[14] M. Andrews and C.M. Savage. Phys. Rev. **A50**, 4535–4537 (1994).

[15] P. Duclos, P. Exner. Rev. Math. Phys. **7**, 73-102 (1995)

[16] I.J. Clark and A.J. Bracken. J. Phys. **A29**, 339–348 (1996).

[17] I.J.Clark and A.J. Bracken. J. Phys. **A 29**, 4527–4535 (1996).

[18] M. Razavy. Phys. Lett. **A228**, 239-242 (1997)

[19] I.J. Clark. J. Phys. **A31**, 2103–2107 (1998).

[20] P. Duclos, P. Exner, B. Meller. Helv. Phys. Acta. **71**, 133–162 (1998).

[21] E. Domany *et al.* Solutions to the Schrödinger equation on some fractal lattices. Phys. Rev. Vol. B28. P. 3110–3123 (1983).

[22] R. Quasti *et al.* J. Phys. Cond. Matt. Vol. 7. P. 811–820 (1995).

[23] N. Zekri *et al.* J. Phys. Cond. Matt. Vol. 7. P. L275 (1995).

[24] George Krylov. Transverse Field Effects and Electron Transport in Quasi-One-Dimensional Systems. Int. J. Nonlin. Phen. Com. Sys. Vol.4, no. 2. P. 129–135 (2001).

[25] Wilfredo Rodriguez. Solution of the time-dependent Schrödinger equation using a continuous Fourier transform. Int. J. Quant. Chem. Vol. 40, no. S25. P. 107-111 (1991); T. R. Taha and M. J. Ablowitz. Analytical and numerical aspects of certain nonlinear evolution equations. II. Numerical, nonlinear Schrödinger equation. J. Comput. Phys. Vol. 55, no. 2. P. 203-230 (1984).

[26] S. Zoldi. Parallel Implementation of the Split-step Fourier Method for Solving Nonlinear Schrödinger Systems. SIAM News. Vol. 32, no.1 (Philadelphia, 2005)

[27] M. A. Belov. Accuracy Estimation of Split-step Fourier method BSU News. S. 1. 2. P. 45-50 (2010).