# Quantum transport in fractal lattices with Coulomb interaction

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In this paper, we study quantum transport, namely, the dynamics of the electron density in a fractal lattice during the propagation of electrons in it. The fractal lattice is composed of nanowires and has the form of a Sierpinski triangle in the direction perpendicular to the direction of electron propagation. The fundamental point is to take into account the Coulomb repulsion of electrons at one lattice site.

**Keywords:** quantum transport, fractals, Hubbard model.

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## 1. Introduction

A fractal is understood as a complex structure with fractional dimensionality that has the property of self-similarity. Fractals are used to describe many phenomena in science and engineering and allow the creation of new devices with improved characteristics.

The influence of fractional dimensionality has been widely studied in terms of diffusion processes by investigating classical random walks in fractal lattices [1]. In distinction from structures with integer dimensionality in fractal objects anomalous diffusion is observed, models of which are described in many works [2–4].

Experimental studies of quantum transport of single photons in a photonic lattice with fractal geometry [5] have been carried out. New materials with fractal structure, in which electron transport [6–8], including tunneling [9], is possible, are being developed and investigated. The quantum conductivity of a two-dimensional electron gas wandering on a Sierpinski [10] carpet is determined.

Note that in the above-mentioned works the one-electron approximation was used. In this work, we will investigate the process of electron transfer in fractal structures in the multielectron approximation, which will allow us to identify features of the properties of materials with such a structure, which can make a significant contribution to the development of new devices.

## 2. Model and solution methods

We consider the propagation of electron density waves in a system consisting of several nanowires, whose cross section is a lattice in the form of a Sierpinski triangle (plane $YOZ$), which has a fractal structure (Figure 1). Let us assume that electrons are launched into our system with a fractal structure and enter the first node (the vertex of the Sierpinski triangle).

Let us write the Hamiltonian of the system using the Hubbard model [11]:

$$H = -\sum_{mj\sigma} \gamma_{mj} a^{+}_{m\sigma} a_{j\sigma} + \sum_{m} U a^{+}_{m\sigma} a_{m\sigma} a^{+}_{m-\sigma} a_{m-\sigma}. \quad (1)$$

Here, $\gamma_{mj} (\approx 0.5\,\text{eV})$ — the jump integral between nodes $m$ and $j$ in the fractal lattice (between nearest neighbors), determined by the distance between nanowires, $U (\approx 10\,\text{eV})$ — the value of Coulomb repulsion of electrons at one node, $a^{+}_{m\sigma} a_{m\sigma}$ — electron birth/annihilation operators at $m$ om node with spin $\sigma$.

Let us further write down the Heisenberg equation of motion:

$$i\hbar \frac{\partial}{\partial t} a_{m\sigma} = [a_{m\sigma}, H]. \quad (2)$$

For simplicity, we consider that the probability of encountering an electron with spin $+\sigma$ and spin $-\sigma$ is the same. By computing the commutator in the right-hand side of equation (2) and going to the continuum limit along the nanowire axis, we obtain an equation describing the dynamics of electron density wave propagation in a fractal lattice:

$$i\hbar \frac{\partial}{\partial t} a_m = -\sum_{j} \gamma_{mj} a_j + U|a_m|^2 a_m - \frac{\hbar^2}{2m_{ef}} \frac{\partial^2 a_m}{\partial x^2}. \quad (3)$$

Here $i$ — imaginary unit, $\hbar$ — Planck's constant, $|a_m(x,t)|^2$ — the probability of finding an electron in a node $m$, $m_{ef} (\approx -10^{-25}\,\text{g})$ — the effective mass of an electron in the nanowire. We consider that the probability of transition along the wire is 5 times higher than in the transverse direction. The transition to the continuum limit along the axis $OX$ is possible when the characteristic size (in this case, the half-width of the Gaussian packet) is much larger than the distance between nodes.

Note that in this work we consider a simple model, taking into account only the short-range interaction between electrons.

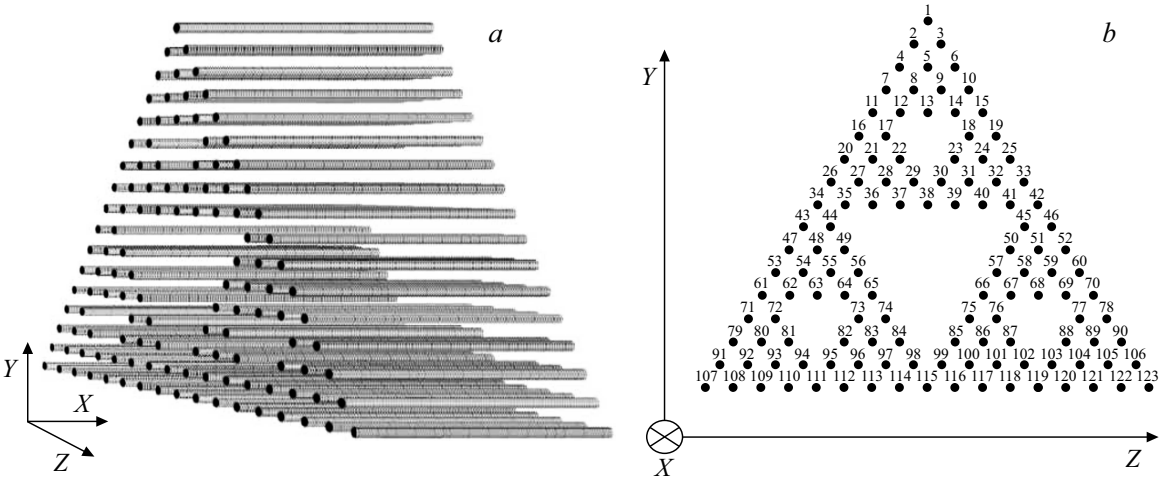


**Figure 1.** Problem geometry: nodes are numbered from top to bottom, left to right.

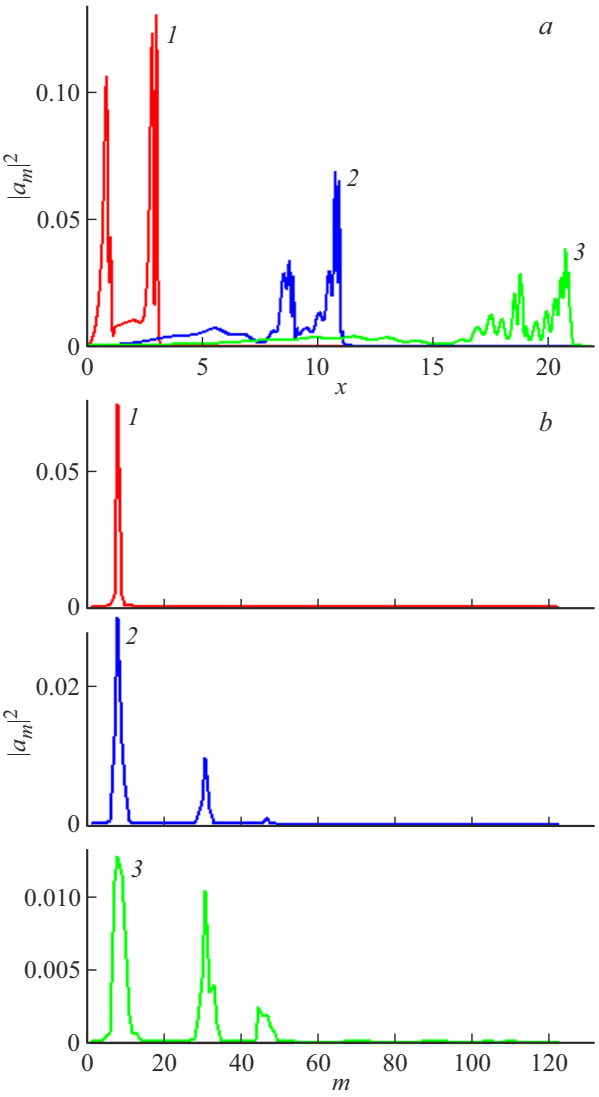


**Figure 2.** *a* — the dependence of the electron density distribution, summed over all nodes, on the coordinates $x$; *b* — the electron density partial distribution as a function of the node number $m$, integrated over $x$: the curve *1* corresponds to $t = 2$, *2* — $t = 10$, *3* — $t = 20$.

Equation (3) was solved numerically (see work [12]) using a graphics processor with initial conditions for the wave function in the form:

$$a_1(x_i, 0) = Q \cdot \exp\left(-\frac{(x_i - b)^2}{g^2}\right), \quad i = 1, \ldots, N, \quad (4)$$

$$a_k(x, 0) = 0, \quad k = 2, \ldots, 162,$$

$$a_k(x_1, t) = a_k(x_2, t), \quad a_k(x_N, t) = a_k(x_{N-1}, t),$$

where $Q$ — the amplitude of the wave packet normalization ($Q = 1$), $g$ — the width of the wave packet of incoming electrons (10 nm), $b$ — the place of maximum of the wave packet (5 nm), $N$ — the number of coordinate steps. The modelling was carried out on nanowires with a length of 200 nm.

The integral characteristics of the electron wave function for different time moments are shown in Figure 2.

From Figure 2, *a*, it can be seen that with the passage of time, the electron density wave propagates along the nanowires with a gradual damping of the amplitude — for the first node and with an increasing — for the node farther away from the apex. At the same time, some electrons transfer to the neighbouring nanowires (Figure 2, *b*). The resulting structure is actually a domain structure. By domains we mean bands with different electron densities. The presence of such a structure may be useful for detecting memory effects in the electronic subsystem of fractal waveguides.

Note that taking into account the Coulomb repulsion of electrons does not change the nature of the evolution of the wave function, manifesting itself only in a change in the value of the electron density within 1–2%.

The dependence of the results on the amplitude of $Q$ was also investigated. It is found to have a non-trivial character, which is manifested by the near-zero interaction at small values of the amplitude of ($Q \leq 0.05$).

Figure 3 shows the Fourier spectra of the wave function. From the above dependences we can conclude that the

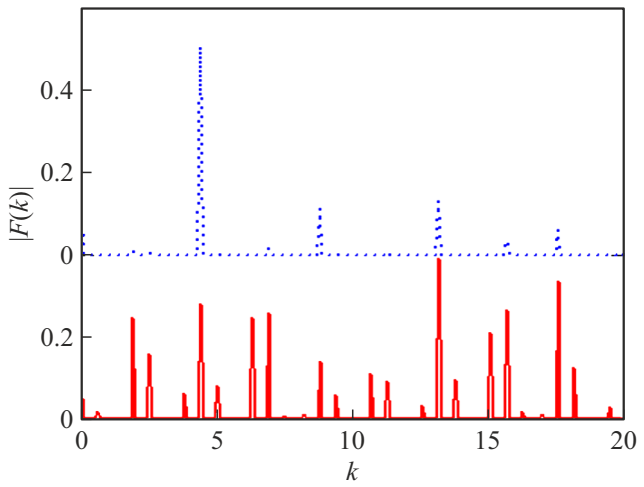


**Figure 3.** Fourier modulus for different nodes of the fractal lattice: solid curve — upper node of Sierpinski triangle, dotted curve — 5th node.

Fourier spectra for different nodes agree, and as a result, frequency-coordinated oscillations are formed in the fractal structure. This, first of all, owes its appearance to the nonlinear summand in (1), which is responsible both for the appearance of higher harmonics and for the synchronization of the spectrum. We note, that such spectra synchronization can be useful in electron density wave splitter devices.

## 3. Conclusion

As a result of this study, it has been revealed that the electron wave functions in fractal structures have the form of localized states and when taking into account the nonlinearity caused by Coulomb repulsion of electrons at one node. It is shown that in a fractal lattice of nanowires there are spectrum-coordinated oscillations of electrons.

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### Conflict of interest

The authors declare that they have no conflict of interest.

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