

THE INCREASE OF THE ELECTRICAL CONDUCTANCE IN NANOSTRUCTURES: A THEORETICAL APPROACH

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Considerând că mișcarea purtătorilor de sarcină are loc pe curbe fractalice, se explică creșterea conductanței electrice în nanostructuri folosind un model extins al teoriei relativității de scală. Rezultă două procese majore responsabile de creșterea conductanței electrice. La scală macroscopică se obține trecerea de la regimul de transport prin structuri necvasiautonomie la cel prin structuri cvasiautonomie, separate de structura 0.7 observată experimental. La scală microscopică procesul este controlat prin intermediul coerenței nano-dilatonilor.

Considering that the charge carrier movements take place on fractal curves, the increase of electrical conductance in nanostructures is explained using an extended model of scale relativity theory. Two major processes result as being responsible for the increase of the electrical conductance. At the macroscopic scale, this increase implies the change of the transport regime of the charge carriers, from transport by means of non-quasi-autonomous structures, to transport by means of quasi-autonomous structures. These two regimes are separated by the experimentally observed 0.7 structure. At the microscopic scale, the process is controlled by means of the nanodilaton's coherence.

Keywords: fractals, nanostructures, charge transport phenomena.

1. Introduction

The transport of charged particles in electronic devices is generally described by kinetic models such as Boltzmann-like equations or macroscopic models of hydrodynamic or diffusion type [1-3]. Due to the ongoing miniaturization of these devices, reaching the nanometric scale, the reliability of these classical models becomes doubtful as quantum effects become important. Since, at an intermediate scale, collision phenomena remain significant, one of the most challenging areas of investigation in semiconductor modeling deals with the setting-up of quantum transport models which take into account scattering effects. Though many works are concerned with the numerical simulation of ballistic quantum transport models for semiconductors (see e.g. [4,5]), a quantum theory of

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collisions is still under development (among other works on the quantum theory of scattering, see *e.g.* [6,7]). Furthermore, several attempts were made to adapt existing classical macroscopic models to quantum mechanics [8-10] but, generally, the link between the so-obtained models and a microscopic quantum description of the particle transport is to a large extent phenomenological.

In solid-state physics and electronics, a large variety of different non-equilibrium phenomena accompany the spontaneous self-assembly of spatial and spatio-temporal patterns. Thus, attention has been paid to thyristor-like semiconductor structures with large active area, as these nonlinear systems with bistable properties show several spatial and spatio-temporal current density patterns. Such semiconductor structures could potentially be used as multi-stable elements for integrated circuits, self-organizing devices for image recognition and image processing.

All these results requires the development of new “scale” physical theories, *i.e.* of fractal space-time type (*e.g.* the scale relativity (SR) model [11,12]), in which the macroscopic scale specific to the classical quantities coexist and it is compatible, simultaneously, with the microscopic “scale” specific to the quantum quantities. Then i) the semi-quantum physical theories, must not be imposed, but are generated as transitions between the interaction scales; ii) the topological dimension and implicitly, the fractal one (for details see [13]) induces new transport mechanisms; iii) the so-called anomalies, *e.g.* the increases of the thermal conductivity in nanostructures, appear as natural phenomenon in the context of material structures self-organization by means of the spontaneous symmetry breaking (for details see [14,15]). In the present paper, considering that the motion of the charge carriers in nanostructures takes place on fractal curves (continuous but non-differentiable curves), the increase of the electrical conductance is explained using an extended model of SR. Such type of movement is the result of the chaotic collective effect induced by all the other charge carriers on the one under discussion.

2. Mathematical model

SR [11,12] is a new approach to understand quantum mechanics, and moreover physical domains involving scale laws, such as chaotic systems. It is based on a generalization of Einstein’s principle of relativity to scale transformations. Namely, one redefines space-time resolutions as characterizing the state of scale of reference systems, in the same way as speed characterizes their state of motion. Then one requires that the laws of physics apply whatever the state of the reference system, of motion (principle of motion-relativity) and of scale (principle of SR). The principle of SR is mathematically achieved by the principle of scale-covariance, requiring that the equations of physics keep their simplest form under transformations of resolution.

According to SR [11,12], a non-differentiable continuum is necessarily fractal and the trajectories in such a space (or space-time) own (at least) the following three properties: i) The test particle can follow an infinity of potential trajectories: this leads us to use a fluid-like description (fractal fluid); ii) The geometry of each trajectory is fractal ([11-13]). Each elementary displacement is then described in terms of the sum, $d\mathbf{X} = d\mathbf{x} + d\boldsymbol{\xi}$, of a mean classical displacement $d\mathbf{x} = \mathbf{v}dt$ and of a fractal fluctuation $d\boldsymbol{\xi}$, whose behavior satisfies the principle of SR (in its simplest Galilean version). It is such that $\langle d\boldsymbol{\xi} \rangle = 0$, $\langle d\boldsymbol{\xi}^2 \rangle = 2D(dt)^{(2/D_F)}$ and $\langle d\boldsymbol{\xi}^3 \rangle = (2D)^{3/2}(dt)^{(3/D_F)}$, where D defines the fractal/non-fractal transition, *i.e.* the transition from the explicit scale dependence to scale independence. The existence of this fluctuation implies introducing new second and third order terms in the differential equation of motion; iii) Time reversibility is broken at the infinitesimal level: this can be described in terms of a two-valuedness of the velocity vector, \mathbf{v}_+ the “forward” speed and \mathbf{v}_- the “backward” speed, for which we use a complex representation, $\mathbf{V} = (\mathbf{v}_+ + \mathbf{v}_-)/2 - i(\mathbf{v}_+ - \mathbf{v}_-)/2$, where the real part defines the classical (differentiable) speed, while the imaginary part refers to the fractal (non-differentiable) character of movement (for details see Refs. [11-16]).

These three effects can be combined to construct a complex time-derivative operator [15,16],

$$\frac{\delta}{dt} = \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla - iD(dt)^{(2/D_F)-1} \Delta + \frac{\sqrt{2}}{3} D^{3/2} (dt)^{(3/D_F)-1} \nabla^3 \quad (1)$$

so that, the first Newton’s principle in its covariant form becomes $\delta \mathbf{V} / dt = 0$, *i.e.*

$$\frac{\delta \mathbf{V}}{dt} = \frac{\partial \mathbf{V}}{\partial t} + \nabla \left(\frac{\mathbf{V}^2}{2} \right) - \mathbf{V} \times (\nabla \times \mathbf{V}) - iD(dt)^{(2/D_F)-1} \Delta \mathbf{V} + \frac{\sqrt{2}}{3} D^{3/2} (dt)^{(3/D_F)-1} \nabla^3 \mathbf{V} = 0 \quad (2)$$

with the special notation $\nabla^3 = \sum_{i=1}^3 \partial^3 / \partial x_i^3$. Therefore, the sum of the local time

dependence, $\partial_t \mathbf{V}$, of the convective term, $\mathbf{V} \cdot \nabla \mathbf{V}$, of the dissipative one, $\Delta \mathbf{V}$, and of the dispersive one, $\nabla^3 \mathbf{V}$ is null in any point of a fractal curve of D_F fractal dimension. This result shows that transport process in nanostructures has hysteretic properties [17-19]: the fractal fluid can be described by Kelvin-Voight or Maxwell rheological model with the aid of complex quantities, *i.e.* the complex speed field, the complex acceleration field etc. and complex structure coefficients, *i.e.* the imaginary viscosity coefficient, $\eta = iD(dt)^{(2/D_F)-1}$, as it will be shown below. We assume that the motion of the fractal fluid is irrotational, $\nabla \times \mathbf{V} = 0$, and then we can choose \mathbf{V} of the form:

$$\mathbf{V} = \nabla \phi = -2iD(dt)^{(2/D_F)-1} \nabla(\ln \psi) \quad (3)$$

In these conditions, Eq. (2) takes the form

$$\frac{\delta \mathbf{V}}{dt} = \frac{\partial \mathbf{V}}{\partial t} + \nabla \left(\frac{\mathbf{V}^2}{2} \right) - iD(dt)^{(2/D_F)-1} \Delta \mathbf{V} + \frac{\sqrt{2}}{3} D^{3/2} (dt)^{(3/D_F)-1} \nabla^3 \mathbf{V} = 0 \quad (4)$$

and ψ satisfies a generalized Schrödinger type equation:

$$D^2 (dt)^{(4/D_F)-2} \Delta \psi + iD(dt)^{(2/D_F)-1} \partial_t \psi + i \frac{\sqrt{2}}{3} D^{5/2} (dt)^{(5/D_F)-2} (\nabla^3 \ln \psi) \psi = F(t) \quad (5)$$

Particularly, when the dispersion is absent, Eq. (4) becomes a generalized Navier-Stoke (GNS) type equation,

$$\frac{\delta \mathbf{V}}{dt} = \frac{\partial \mathbf{V}}{\partial t} + \nabla \left(\frac{\mathbf{V}^2}{2} \right) - iD(dt)^{(2/D_F)-1} \Delta \mathbf{V} = 0 \quad (6)$$

with imaginary viscosity coefficient, $\eta = iD(dt)^{(2/D_F)-1}$, and from here, using Eq. (3), the Schrödinger type equation results,

$$D^2 (dt)^{(4/D_F)-2} \Delta \psi + iD(dt)^{(2/D_F)-1} \partial_t \psi = 0 \quad (7)$$

Moreover, for $D = \hbar/2m$, with \hbar the reduced Planck's constant, m the rest mass of the test particle and for the fractal dimension, $D_F = 2$, *i.e.* for movements on fractal curves of Peano type [11,12], the previous equation is reduced to standard Schrödinger equation.

In the particular case when the dissipation is absent, Eq. (4) becomes a generalized Korteweg de Vries (GKdV) type equation,

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} + \frac{\sqrt{2}}{3} D^{3/2} (dt)^{(3/D_F)-1} \nabla^3 \mathbf{V} = 0 \quad (8)$$

Let us choose the function $\psi = \sqrt{\rho} \exp(iS)$, with $\sqrt{\rho}$ the amplitude and S the phase. By substituting the complex velocity field (3), $\mathbf{V} = \mathbf{v} + i\mathbf{u} = 2D(dt)^{(2/D_F)-1} \nabla S - iD(dt)^{(2/D_F)-1} \nabla \ln \rho$ in Eq. (8), and separating the real and imaginary parts, it results the equation system,

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + \nabla \left(\frac{\mathbf{v}^2}{2} - \frac{\mathbf{u}^2}{2} \right) + \frac{\sqrt{2}}{3} D^{3/2} (dt)^{(3/D_F)-1} \nabla^3 \mathbf{v} &= 0 \\ \frac{\partial \mathbf{u}}{\partial t} + \nabla(\mathbf{v} \cdot \mathbf{u}) + \frac{\sqrt{2}}{3} D^{3/2} (dt)^{(3/D_F)-1} \nabla^3 \mathbf{u} &= 0 \end{aligned} \quad (9a,b)$$

In the differentiable case, *i.e.* at the macroscopic scale, $\mathbf{u} = 0$ or $\rho = \text{const.}$, and for the one-dimensional case, with the dimensionless parameters,

$\phi = (j/j_0) = q\rho v/j_0$, $\tau = \omega_0 t$, $\xi = k_0 x$, and the normalizing conditions $(k_0 j_0 / 6q\rho\omega_0) = \sqrt{2}D^{3/2}(dt)^{(3/D_F)-1}(k_0^3/3\omega_0) = 1$, Eqs. (9a,b) take the form,

$$\partial_\tau \phi + 6\phi \partial_\xi \phi + \partial_{\xi\xi\xi} \phi = 0 \quad (10)$$

According with [20] this equation has the solution,

$$\phi(\xi, \tau) = 2a \left(\frac{E(s)}{K(s)} - 1 \right) + 2a \cdot cn^2 \left\{ \frac{\sqrt{a}}{s} \left[\xi - 2a \left(\frac{3E(s)}{K(s)} - \frac{1+s^2}{s^2} \right) \tau + \xi_0 \right]; s \right\} \quad (11)$$

where cn is the Jacobi's elliptic function of s modulus [21], $K(s), E(s)$ are the elliptic complete integrals [12], and ξ_0 constant of integration. As a result, at the macroscopic scale, the electrical charge transport in nanostructures is achieved by one-dimensional cnoidal oscillation modes of the charge current density. This process is characterized through the normalized wave length,

$$\lambda = \frac{2sK(s)}{\sqrt{a}} \quad (12)$$

- see Figure 1a, the normalized phase speed

$$v_f = 4a \left[3 \frac{E(s)}{K(s)} - 1 - \frac{1}{s^2} \right] \quad (13)$$

- see Figure 1b, and the normalized group speed,

$$v_g = 4a \left[3 \frac{E(s)}{K(s)} - 1 - \frac{1}{s^2} + 3 \frac{E^2(s) + 2(s-1)E(s)K(s) - (s-1)K^2(s)}{E(s)K(s) + K^2(s) - sK^2(s)} + \frac{2(s-1)K(s)}{s^2[E(s) + K(s) - sK(s)]} \right] \quad (14)$$

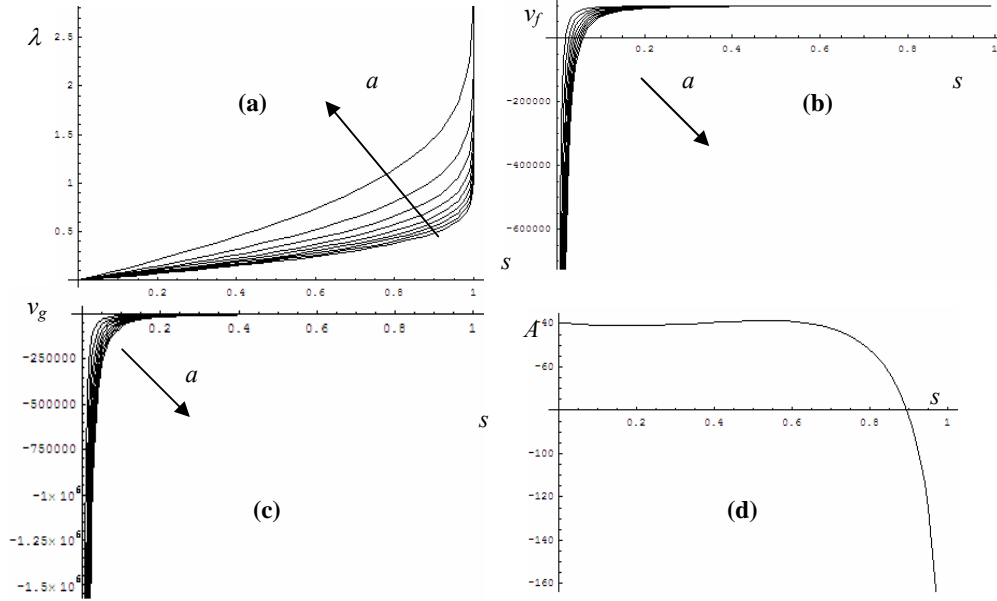
-see Figure 1c. In such conjecture, the followings result:

i) by eliminating the parameter a from relations (12) and (13), one obtains the dispersion relation, $v_f \lambda^2 = A(s)$, with $A(s) = 16 \left[3s^2 E(s)K(s) - (1+s^2)K^2(s) \right]$. In Figure 1d the quantity $A(s)$ is numerically evaluated. We observe that only for $s = 0 \div 0.7$, $A(s) \approx \text{const.}$, and the dispersion equation takes the form, $v_f \lambda^2 = \text{const.}$;

ii) the parameter s becomes a measure of the electric charge transfer in nanostructures. Thus, for $s \rightarrow 0$, λ , v_f and v_g are small, while for $s \rightarrow 1$, λ , v_f and v_g are high — see Figures 1a-c;

iii) the one-dimensional cnoidal oscillation modes contain as subsequences: ii₁) for $s = 0$ the one-dimensional harmonic waves and ii₂) for $s \rightarrow 0$ the one-dimensional waves packet. These two subsequences describe the electric charge transport in a non-quasi-autonomous regime (for details see [17-19]). ii₃) For $s = 1$, the solution (11) becomes a one-dimensional soliton, while ii₄) for $s \rightarrow 1$ the one dimensional solitons packet results. These last two

subsequences describe the electric charge transport in a quasi-autonomous regime (for details see [17-19]). Therefore, these two regimes (non-quasi-autonomous and quasi-autonomous) are separated by the 0.7 structure, a value in agreement with the experimental data [22].



Figs. 1a-d: The dependences on s of the (a) normalized wave length λ , (b) normalized phase speed v_f , (c) group velocity v_g (various values of the parameter a), and (d) of the quantity A

The previous results show, through the normalized group speed (14), an increase of the charge transport in nanostructures by means of quasi-autonomous structures. They can provide a possible explanation of the anomalous increase of the electrical conductance that was experimentally observed in [18,19].

Let us study now the previous phenomenon in the non-differential case, *i.e.* at microscopic scale. This can be achieved by the substitutions $\phi = (v_f/4)f^2$ and $i\eta = (v_f/4)^{1/2}(\xi - v_f\tau)$ in Eq. (10). By an adequate choice of the integration constants, it becomes, $\partial_{\eta\eta}f = f^3 - f$, *i.e.* a Ginzburg-Landau type equation [23]. The followings result:

- i) The η coordinate has dynamic significations and the variable f has probabilistic significance –for details see [11,12]. The space-time becomes fractal;
- ii) According to [24] we can build a field theory with spontaneous symmetry breaking. The fractal kink solution,

$$f_k(\eta) = f(\eta - \eta_0) = \tanh[(\eta - \eta_0)/\sqrt{2}] \quad (15)$$

spontaneously breaks the “vacuum” (the minimum energy states of the system) symmetry by tunneling, and generates coherent structures. This mechanism is similar with the one of superconductivity [25];

iii) the normalized fractal potential take a very simple expression which is directly proportional with the density of states of the fractal fluid,

$$Q = -(1/f)(d^2 f d\eta^2) = (1 - f^2). \quad (16)$$

When the density of states, f^2 , becomes zero, the fractal potential takes a finite value, $Q = 1$. The fractal fluid is normal (it works in a non-quasi-autonomous regime) and there are no coherent structures in it. When f^2 becomes 1, the fractal potential is zero, *i.e.* the entire quantity of energy of the fractal fluid is transferred to its coherent structures. Then the fractal fluid becomes coherent (it works in a quasi-autonomous regime). Therefore, one can assume that the energy from the fractal fluid can be stocked by transforming all the environment's entities into coherent structures and then 'freezing' them. The fractal fluid acts as an energy accumulator through the fractal potential (16);

iv) substituting (15) in (16) the fractal potential (16) becomes a soliton at nano scale,

$$Q = \sec h^2 \left[(\eta - \eta_0) / \sqrt{2} \right] \quad (17)$$

and can be associated with a nanodilaton (for details on this concept see [17-19]). In certain conditions of an external load (*e.g.* an external stress) the nanodilatons break down (blow up) and release its energy. As a result, the nanostructure energy unexpectedly increases.

3. Conclusions

Considering that the charge carrier movements take place on fractal curves, the electric charge transport is studied in an extended model of SR. It results: i) An equation of motion is deduced for the complex speed field, where the local complex acceleration, convection, dissipation and dispersion are reciprocally compensating. Using this equation, for the irrotational movement the generalized Schrödinger equation is obtained. The absence of the dispersion implies a generalized Navier-Stokes type equation, and from here, for the irrotational movement and fractal dimension $D_F = 2$, the usual Schrödinger equation resulted; ii) The absence of dissipation implies a generalized Korteweg de Vries type equation. In the one-dimensional macroscopic case, two flowing regimes (quasi-autonomous and non-quasi-autonomous) of the charge carriers are evidenced, the separation between them are being made by the 0.7 structure that is experimentally observed. In such conjecture, the increase of the electrical conductance in nanostructures is connected with the increase of the group velocity at the passage from non-quasi-autonomous to quasi-autonomous regime; iii) At

microscopic scale, the electrical conductance increase is controlled by means of the nanodilaton coherence. When the external field exceeds a critical value, the nanodilaton which stock the energy break down and simultaneously release the energy to the environment.

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