"ALEXANDRU IOAN CUZA"

DEPARTMENT OF PHYSICS

CONTRIBUTIONS TO THE STUDY OF TRANSPORT MECHANISMS IN NANOSTRUCTURES

- PhD Thesis -

Candidate:

STANA-ROXANA ADRIANA

Supervisor:

Prof. Dr. AGOP MARICEL

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DOCTORATE THESIS CONTENTS

Key words: thermal transfer, nanostructure, mechanism, electrical conductivity, Casimir force, fractal, theory of space.

The current paper, titled ***"Contributions to the Study of the Transport Mechanisms in Nanostructures"*** has the purpose the studying of some elements of nonlinear dynamics (chaos, self-structuring, spontaneous symmetry breaking, fractals, etc.) within the (thermal, charges) transport processes in nanostructures.

It is structured in 3 chapters, introduction, general conclusions and bibliographical references. Out of the 101 references, 11 of them belong to the author of this thesis, 3 of the articles having Impact Factor Rankings.

In the first chapter, called **"Thermal Transfer Mechanisms within Nanostructures",** a new mathematical model is being created, regarding the thermal transport in nanostructures, taking into account that it is produced on "thermal" and non-differentiable curves ("thermal fractal curves"). With this opportunity, we will prove that standard thermal transfer mechanisms, as well as the convective thermal transport, the phononic thermal transfer, the thermal transport through other patterns, and others, are sequences of a unique transfer mechanism which takes place at different scale levels.

The second chapter, ***"Exotic Mechanisms of Electrical Conductivity in Nanostructures"***, allows us to study the Hall Quantum Effect in graphene from the perspective of a spontaneous symmetry breaking field theory, within a fractal time-and-space, and the research of the fractional Hall Effect from a Toda bi-dimensional network perspective. Within this framework, concepts like intrinsic anisotropy, forbidden energy band, filling factor, etc., appear as if they are the same "faces" of the same "mask" generated by using the non-differentiability notion.

The third chapter, named ***"Contributions to the Study of the Casimir Effect by Using the Fractal Theory of Space"***, provides a new method for calculating the Casimir force required for a rectangular cavity with a quantic fluid, non-differentiable, bi-dimensional, Newtonian, made up from assimilated quasiparticles with vortex type objects. By self-structuring, due to imposed constraints of the walls presence, forces are being generated. The obtained results are in agreement with the regularization calculus by using the Abel-Plana relation.

GENERAL CONCLUSIONS

The approach of the dynamic nanostructures based on the non-differentiability of the sizes that describe it, of the time and resolution coordinates dependency that is, implies unitary mechanisms of transport phenomena analysis. Thus, in the case of the dissipative approximation of the thermal transfer, the conductivity fractal mechanism is distinguished, which for the Peano type of trajectories of the entities of the nanostructure is reduced to the standard one. In the case of the dispersive approximation of the thermal transfer within nanostructures, a phononic type of mechanism is simulated, with two working conditions, while through fractalization conductive mechanisms are emulated through patterns (a thermal type of pairs).

The electrical conductivity in graphene implies “exotic” mechanisms which are generated through either the full Hall Quantum Effect, or the fractional Hall Quantum Effect. The first of them is implied by a spontaneous symmetry breaking field theory, while the second of them is driven by the dynamics of bi-dimensional Toda networks.

The Casimir force calculus, by using the relativity theory formalism on a scale based on the hypothesis that the void from the Casimir cavities, initially a quantic fluid, non-differentiable, bi-dimensional, without coherence, newtonian, made up from quasiparticles, which can be assimilated with a vortex type of objects, becomes through constraints a coherent fluid, it reflects the hypothesis validity of the movement on continuous and non-differentiable curves. The fact that matching patterns similar to those known one are obtained in particular instances allows the mathematic formalism to be extended when induced by the relativity theory on a level of the interaction study on a Planck and a nuclear scale.

The fact that phenomena on various scales (the thermal convection scale, the electrical conductivity scale, the nanoscale, the mesoscale etc.) can be approached through the hypothesis of the movement of entities (particles, quasiparticles etc.) from continuous curve and non-differentiable complex systems (particularly the fractal curves) specifies that the geometry of nature is not an Euclidian one, a Riemannian one, but a non-differentiable one. As Mandebrot said, the geometry of nature has to be the fractal one.

A thermal transfer mechanism has been obtained within the nanostructures, taking into account the fact that the thermal movements of the quasiparticles from the nanostructures take place on continuous and non-differentiable curves (fractal curves). These have been called “thermal trajectories”;

In the most general case, the thermal transfer equation specifies the fact that the local temporal variation, the self-convection, self-dissipation and the self-dispersion create a balance in any point of the “thermal trajectory”. Moreover, the behavior of the fractal fluid is viscous or hysteretic, in the sense that it displays memory features;

The separation of the thermal movements on interaction scales specifies for the non-differentiable interaction scale the fact that the local temporal variation, the self-convection, self-dissipation and the self-dispersion of the thermal field create a balance at any point of “the thermal trajectory”, while on the fractal interaction scale only the fractal self-convection and the thermal field dissipation create a balance in any point of the thermal trajectory;

In the case of the dissipative approximation of the thermal transfer (the self-convection and self-dissipation are dominating when compared to self-dispersion), on the differentiable scale, the local temporal variation and the thermal field self-convection create a balance in any point of the thermal trajectory, while on a fractal scale, the fractal self-convection and self-dissipation of the very same thermal field make a balance in any point of the "thermal trajectory";

Through the unification of the interaction scales, the thermal transfer equation associated with the fractal/non-fractal transition is induced. As a result, the thermal transfer fractal equation is obtained, while for synchronous movements on the two scales of interaction on the Peano type of "thermal curves" the standard thermal transfer equation is applied.

The numerical solutions of the thermal transfer fractal equation for a plane symmetry specify that in the absence of a conductive wall a thermal perturbation is dissipated due to the rheological properties of the fractal environment, but in the presence of a conductive wall, the thermal perturbation is regenerated at the wall.

The entire thermal conductivity of a nanofluid is being proven to be directly proportional to the volume fraction of the nanoparticle and the report of the coefficients of the nanoparticle-fluid thermal transfer, and inversely proportional to the nanoparticle radius, in the case where nanoparticles are spheres;

In the case of the dispersive approximation of the thermal transfer (the self-convection and self-dispersion are dominating when compared to self-dissipation), on a differentiable scale, the local temporal variation, the self-convection and the self-dispersion of the thermal field create a balance in any point of the "thermal trajectory", while on the fractal scale, the fractal self-convection of the same thermal field is null.

Through the unification of the interaction scales, a thermal transfer equation associated with the fractal/non-fractal transition is induced. The one-dimensional analytical solution of this equation specifies that the thermal transfer is done through spatial and temporal cnoidal oscillation modes of the thermal field with a wavelength and phase speed which are well defined and depend on the thermal field amplitude as well as on the non-linearity degree;

For small non-linearity degrees the cnoidal oscillation modes degenerate into harmonic thermal waves and harmonic thermal wave packets, while the high non-linearity cnoidal oscillation modes degenerate in thermal solitons and thermal soliton packets;

Through the elimination of the amplitude between the typical wavelength and the phase speed, the thermal dispersion relation is obtained. From its analysis, two thermal transfer conditions come out, the thermal non-quasiautonomous one (through thermal harmonic waves and thermal harmonic wave packets) and the thermal quasiautonomous one (through thermal solitons and thermal soliton packets). These thermal transfer conditions are separated through the 0.7 non-linearity degree which was determined through experiments.

The assimilation of the cnoidal oscillations in a non-linear oscillators Toda network involves the simulation of the thermal transfer through a phononic type of mechanism. Within such a framework the two thermal transfer conditions can be associated to two types of phononic specters, the optical and the acoustical one.

Through the fractalization of the thermal transfer conditions from the approximate dispersion, a Ginzburg-Landau type of equation is obtained. Within such a framework, the thermal field gets statistical significance and the field variable, initially a static one, becomes a dynamic variable. Moreover, the thermal transfer mechanisms are of a collective type through Cooper "thermal pairs" and are described by their specific parameters, like the breaking time of the "thermal pair", the relative concentration of the "thermal pair", the relative thermal conductivity etc. These parameters do no show discontinuities for lower degrees of non-linearity, but they are present in high non-linearity degrees.

The self-structuring process of the fractal fluid in the “thermal pairs” is controlled by a fixed thermal “fractal potential”. This potential which is directly proportional to the pair density tends to be one as a value when the pair density is null, and tends to be zero when the pair density is one as a value. Thus, the transition is made from incoherence into coherence, which implies that the energy of the fractal fluid can be stored through the environment entities transformation into coherent structures (Cooper “thermal pairs”), those being then “frozen”. This energy could explain, for example, the thermal anomaly of the nanostructures.

PERSPECTIVES

a. A unique transfer mechanism is suggested by the movement of the quasiparticles on fractal trajectories. Within such a framework, the Lagrangean formalism keeps its validity both in its relation to temporal and spatial coordinates, as well as in resolution scales.

b. Admitting a minimal coupling between the scalar potential of the complex field of speeds and the vectorial potential of the magnetic field, the Lagrangean and the Euler-Lagrange equations are built, the equations being associated for a cylindrical symmetry. The obtained analytical solutions are finite in the potential vector, but the divergences in the scalar potential within the asymptomatic limit result in $\mathbf{r}\to\infty$. The indeterminacy increases by redefining the Lagrangean which now shows a spontaneously broken symmetry through the addition of a self-interaction to the mass term. Practically, we are talking in terms of a spontaneous breaking field theory of a Nielsen-Olsen symmetry type.

c. Out of the pattern of spontaneous breaking results he symmetry of the entire magnetic flux quantification and the entire Hall resistance quantification, respectively the Hall conductivity. The last situation is obtained by using both the Hall potential difference expression, as well as the explanation of the number of states on each Landau level.

d. Assuming that in the one-dimensional case the load transfer is accomplished through cnoidal oscillation modes of a complex field of speeds, the appliance of these results on a bi-dimensional space implies the dynamics of a bi-dimensional quasiparticles network, which are associated with a vortex type of objects (a Toda bi-dimensional type of network). These quasiparticles, initially dynamically non-coherent, in the absence of the magnetic field, become dynamically coherent (correlated in phases and amplitudes) in the presence of such a field. The coherence on the level of vortex networks is shown by the self-structuring of vortex streets, simultaneously, along the Ox axis, as well as on the Oy axis. Mathematically speaking, we will describe the above mentioned dynamics through a complex potential of speeds, and, moreover, through its derivation in relation to a dynamically complex variable, through a complex impulse. The simultaneous placing of the conditions of the degeneration of the real part of the complex impulse, in relation to the smallest and the biggest non-linearity degree, generates impulse components which induce measurable ‘effects’. By applying the specific impulse rotor, the non-null vortex field is obtained along the Oz axis, whose mediation in relation to the elementary cell is responsible for the intrinsic anisotropy of the nanostructure. Moreover, through multiplication of the vortex field mediated on the elementary cell with the elementary cell area, we can obtain elements which specify both the filling factor from the Hall Quantum fractional effect, as well as the forbidden energy bands.

i. A new method for calculating the Casimir force is proposed, by using the TRS, totally different from either the quantum fields theory by using the appropriate Green functions for describing the geometry, the dimensional regularization by using the Riemann's Zeta functions and the analytical continuities, or the Euler-Maclaurin integrals formalism;
ii. For the achievement of the proposed purpose, we admitted that the void from the Casimir cavities is a quantic fluid, non-differentiable (the entities of the void are moving on fractal curves), bi-dimensional, incoherent, (there are no correlations between the amplitude and the phases of the entities of the void), Newtonian. Moreover, the entities of the void are assimilated with a vortex type of objects;
iii. The non-differentiable fluid becomes coherent (there are correlations between the amplitudes and the phases of the entities of the void) due to the imposed constraints by the presence of walls;
iv. The mathematical formalism used here is identical with the one from Chapter 2, namely the one of the Toda bi-dimensional networks. The only difference here is that once the complex field of speeds (identical with the one in Chapter 2) is defined, the pressure gradients along the Ox axis, respectively the Oy axis, are calculated as the differences between the dissipative and the convective fields at the fractal-non-fractal transition level, along the above mentioned axes;
v. In the case of a rectangular Casimir cavity the degenerations in relation to the biggest and smallest non-linearity degree must be used simultaneously. Thus, the force expression depends on three parameters (two m and n integers and the relation r=b/a) and it specifies the fact that for close m and n, the force against the Casimir rectangle is always negative, and it decreases exponentially with the increase of r, while for 'asymmetrical' m and n parameters, the Casimir force has both negative and positive fields and it increases exponentially with the increase of r;
vi. For particular values of m, n and r, the calculus of the Casimir force for a rectangular geometry is in agreement with the regularization calculations by using the Abel-Plana formula.

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