Advanced quantum and statistical methods for mesoscopic systems, with applications in the construction of ultra-sensitive devices

PROJECT TITLE: Advanced quantum and statistical methods for mesoscopic systems, with applications in the construction of ultra-sensitive devices
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Project manager: Dragoş-Victor Anghel
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In the following we list the most important results of the project.

1 Ultra-sensitive devices

Advanced theoretical methods proposed and developed during the project have allowed us to bring out physical effects important for the design of ultra-sensitive micro- and nano-sensors for various external fields (magnetic, electromagnetic radiation, heat, etc.).

1.1 Magnetic properties of nano-particles

Application of the new method for the description of quantum statistical thermodynamics of excitations in finite crystals has lead to the generalized form of Bloch law valid for the temperature dependent magnetization of magnetic nanoparticles (NP). The method has been developed in the framework of the Heisenberg spin model and takes into account the effects of size, shape and surface boundary conditions. This description establishes explicit connection between the behavior of magnetization and the microscopic parameters of the model in contrast to the existing semi-empirical description of experimental data. In particular, we show for a specific example that the latter may be misleading and grossly overestimates magnetic softening in nanoparticles believed to be the cause of lower magnetization in free standing nanoparticles as compared to bulk materials. The theory clarifies why the usual $T^{3/2}$ dependence appears to be valid in some nanostructures, while large deviations are a general rule. We demonstrate that combination of geometrical characteristics and coupling to environment can be used to efficiently control magnetization and, in particular, to reach a polarization even higher than in the bulk material, an effect important for magnetic sensing. Thus, by embedding an initially unpolarized at a given temperature free NP into a polarizable medium it is possible to induce a magnetic moment which can exceed even the bulk value, this effect is strongly enhanced by shape anisotropy so that spontaneous magnetization can take place in an abrupt way: from zero to almost complete saturation. For an asymmetric shape one can increase or even decrease the magnetization of a free standing NP depending on the size and shape of the contact area, suggesting an interesting possibility of controlling magnetization. This introduces a new

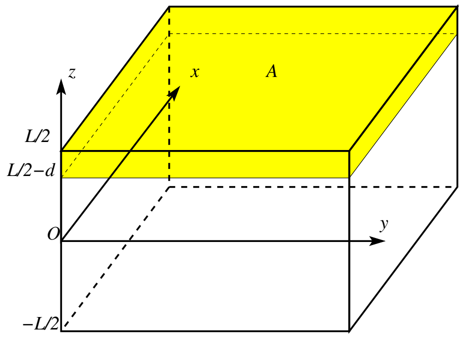

Figure 1: The schematic model of the system. On a dielectric membrane with parallel surfaces perpendicular on the z axis is deposited an uniform metallic film. The surfaces of the membrane cut the z axis at $-L/2$ and $L/2-d$, wheres the upper surface of the film cuts the z axis at $L/2$. In the (x, y) plane the area of the device is A ($\gg L^2$) (from Ref. [21])

physical mechanism specific to nanosized objects, namely, that in the case of non-uniform surface coupling suppression of spin fluctuations on a part of the surface can be prevailed by the enhanced fluctuations of the other spins of the sample, see Papers [1,4,5,7,8,15].

1.2 Nano-detectors for infrared and far-infrared radiation

Important new properties of nanosized systems have also been revealed in the context of modern ultra-sensitive microscopic power detectors (radiation, particles, heat), i.e. microbolometers. Such devices usually contain three essential parts: the absorber, the thermometer and the cooler. Their applications span from cooling microchips in quantum technology to ultra-sensitive microwave radiation detection in astronomy, while low temperatures are commonly required for a top performance of such detectors. The main active element in each of the parts is an ultrathin metal stripe supported by a thin insulating membrane (Fig. 1). The energy flow in such systems depends to a great extent on the properties of phonons and their interaction with electrons. Earlier experiments on the electron phonon energy transfer (Karvonen, Maasilta, 2007) have suggested the possibility of a qualitatively different behavior below certain temperature T^* in the sub-Kelvin region for some tens of nm thick metal film, where a "dimensional crossover" of the phonon spectrum takes place. We have developed a theory [21,22], taking into account the situation existing in real devices and, in particular, were able to give a quantitative explanation of the observed behavior (see Fig. 2). We demonstrate that the phonons dominating the physics at such temperatures and sizes are effectively confined by a quasi-2D "plate" geometry of the film and correspond to the elastic eigenmodes known as Lamb's dilatational and flexural modes. Their interaction with electrons is enhanced orders of magnitude as compared to bulk (see Fig. 3). Furthermore, the very sharp dependence of the heat power on the thickness of the film allows one to control the coupling between electrons and phonons by changing the thickness of the film.

Although the general rule is that interaction and energy transfer is enhanced for thinner films, the situation is more complex in real composite structures. We have shown for a specific structure of a Cu film deposited on an insulating membrane SiN_x studied experimentally that the dependence on thickness become non-monotoneous and a stronger energy transfer between electrons and phonons may occur also for a thicker metal-insulator structure. A crucial role in this effect is due to the phonon behavior in a composite layer, which was found in an explicit form. These results can guide the design of more efficient microcoolers and microbolometers by optimizing the control over the electron-phonon interaction and phonon propagation, see Papers [21,22].

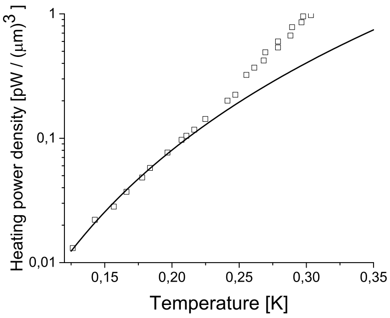

Figure 2: The power density of the electron-phonon heat transfer–comparison of the theoretical results (solid line) with the experimental results (squares) from Karvonen and Maasilta, Phys. Rev. Lett. **99**, 145503, 2007 (from Ref. [23]).

The study of the interaction between phonons and dynamical defects in materials have been continued in Ref. [11], to show that the model employed (and which was also proposed by DVA and collaborators in Phys. Rev. B **75**, 064202, 2007) is generally applicable to such phenomena and therefore gives a correct description of the supporting amorphous membrane.

1.3 Nano-devices with applications in spintronics

We investigated the spin filtering effects in graphene nanoribbons, where inclusions of hexagonal boron nitride were introduced together with substitutional magnetic impurities. The embedded Mn-doped boron nitride regions serve as quasi-0D islands of diluted magnetic semiconductor in the otherwise metallic graphene nanoribbon. Our first principle approach based on non-equilibrium Greens functions gives the polarization of the spin current for structures with one or two Mn impurities as a function of the applied bias. For the two impurity case, ferromagnetic and antiferromagnetic spin configurations of the magnetic impurities are considered. The spin resolved current indicates that the analyzed structures are suitable for spin filter applications or for spin current switching devices (Ref. [6]).

Spin transport properties of magnetic nanowire systemsatomic-sized AlN nanowires with additional Mn impurities were investigated employing ab initio constrained spin density functional theory calculations and non-equilibrium Greens functions formalism. The analyzed nanowire

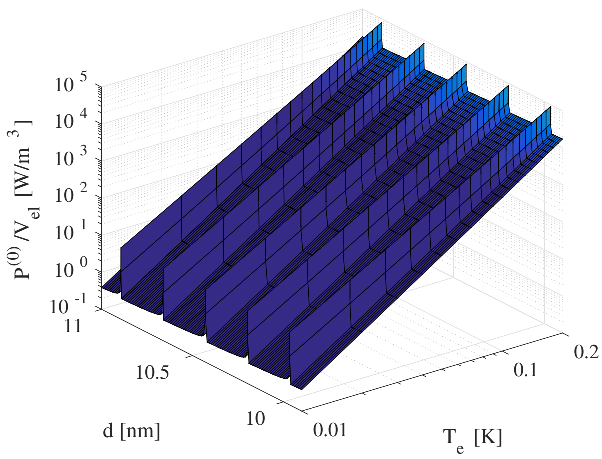

Figure 3: The heat flux from electrons system to the lattice, normalized to the volume of the metallic film, $P^{(0)}/V_{el}$ for $L = 100$ nm (from Ref. [22]).

structures exhibit a stress-induced phase transition, between würtzite and graphite-like configurations. In these quasi-one dimensional systems, the surface states ensure the basic prerequisite in establishing spin and charge transfer, by reducing the relatively large bandgap of the group III nitride semiconductor. The results show in how far this phase transition affects the surface states, focusing on the consequences which appear in the spin-filtering processes (Ref. [10]).

The transport properties of single ferrocene molecules connected to nanoscopic gold electrodes were investigated in the framework of density functional theory (DFT) calculations using the non-equilibrium Green's function formalism. Our setup describes a molecular rotor, where one cyclopentadienyl (Cp) ring of the ferrocene molecule is fixed by the two electrodes, while the second ring is able to rotate. For small enough rotation energies the barrier between the eclipsed and staggered conformations of the ferrocene molecule ensures the functionality of a molecular oscillator. The changes in the transmission function introduced by the relative rotation angle between the two Cp rings are analyzed in both linear and non-linear bias regimes. For larger rotation energies, the device works in the spinning mode. The real time behavior of the nanomechanical device is investigated using DFT-based molecular dynamics, which shows its feasibility for applications in the terahertz regime. In the oscillating mode the natural frequencies are determined, while the spinning mode shows a remarkably reliable behavior with increasing rotation energy (Ref. [16]).

The transport properties of fulgide-based photochromic switches were investigated in the framework of density functional theory calculations. In our setup, light activated furyl fulgide molecules are coupled to nanoscopic metallic electrodes. The electrocyclization process under UV light converts the open-ring into a closed-ring conformation. Conversely, the reverse process takes place by visible light illumination. The switching properties are first analyzed in the linear bias regime revealing a high conductance ratio between the open and closed configurations. The robustness of the results is investigated by analyzing comparatively two compounds from the same family, namely furyl and thiophene fulgides. For both systems, at finite applied bias, one can establish three working regimes, which correspond in turn to a photochromic switch, a negative differential conductance element or to a logical inverter, pointing out the versatility of the considered fulgide-based devices (Ref. [18]).

1.4 Applications of fractional exclusion statistics

The nanodetectors analyzed during this project are formed in general of several qualitatively different subsystems. In each subsystem, the constituent quasiparticles interact with each-other and there is also heat and quasiparticle exchange between different subsystems. For these reasons we developed theoretical tools for the description of the dynamics of such systems, based on fractional exclusion statistics (FES), which is a generalization of Pauli exclusion principle. Using FES, we could transform systems of interacting particles into systems of ideal particles, in a very general way and without using approximations. Our application of the fractional exclusion statistics (FES) to the description of interacting particle systems (Refs. [2,3,11,13,14,17,24]) has been successful. In a series of publications, some results obtained earlier by DVA have been called **Anghel's rules** [of FES] (see for example Phys. Rev. E **85**, 011144, 2012; J. Stat. Mech. P04018, 2013; J. Stat. Mech. P04008, 2014). Below we list the main results obtained during the project.

We developed a model based on the fractional exclusion statistics to describe systems with localized states. The local distribution of the energy levels is captured in the formalism by including the positions in the definition of the species. The particle distributions on the energy axis, as well as in the real space are determined for test-case systems with a peak/dip profile in the local density of states (Conf. Proc. [5]).

We described a mean field interacting particle system in any number of dimensions and in a generic external potential as an ideal gas with fractional exclusion statistics (FES). We define the FES quasiparticle energies, we calculate the FES parameters of the system and we deduce the equations for the equilibrium particle populations. The FES gas is ideal, in the sense that the quasiparticle energies do not depend on the other quasiparticle levels populations and the sum of the quasiparticle energies is equal to the total energy of the system. We prove that the FES formalism is equivalent to the semiclassical or Thomas Fermi limit of the self-consistent mean-field theory and the FES quasiparticle populations may be calculated from the Landau quasiparticle populations by making the correspondence between the FES and the Landau quasiparticle energies. The FES provides a natural semiclassical ideal gas description of the interacting particle gas (Ref. [11]).

Vice-versa, an "ideal" FES system may be transformed back, into a gas of quasiparticles which obey Bose or Fermi distributions; the energies of the newly defined quasiparticles are calculated starting from the FES equations for the equilibrium particle distribution. In this way we established a two-way correspondence between the two types of statistics (see Ref. [13]).

We proposed a drift-diffusion model for systems which obey fractional exclusion statistics (FES), in a framework where the species include classical degrees of freedom such as positions. The transition rates are calculated and the relation between the step and acceptance probabilities on one hand and the diffusion and drift processes on the other hand are established. A Monte Carlo scheme is implemented on a prototypical double-junction system of particles with screened Coulomb interactions. In our approach the properties of interacting quantum gases are locally included using the FES methodology. The model is suitable to describe transient as well as stationary regimes (Conf. Proc. [10]).

As an application of FES to the BCS theory we describe a superconductor as an ideal gas of quasiparticles with fractional exclusion statistics (FES). For this we redefine the quasiparticle energies in such a way that the energy of the superconductor (up to a constant which is the energy of the superconductor at zero temperature) is the sum of quasiparticle energies. The new FES quasiparticles exhibit the same energy gap as the BCS quasiparticles, but have a density of states which is finite at any quasiparticle energy. We also discuss the effect of the remnant electron-electron interaction (electron-electron interaction beyond the BCS pairing model) and show that this can stabilize the BCS condensate, increasing the critical temperature (Ref. [24]).

1.5 Revision of the BCS theory

An important part of the nanodetectors discussed in Section 1.2 is a superconducting film. The detectors functionality is determined by normal metal-insulator-superconductor (NIS) tunnel junctions, which are used both, as micro-coolers and thermometers. This motivated us to study in more detail the superconducting phase and we arrived to a revision of the BCS theory, published in Ref. [25]. In this paper we studied the effect of the chemical potential on the results of the BCS theory of superconductivity. We assumed that the pairing interaction is manifested between electrons of single-particle energies in an interval $[\mu - \hbar\omega_c, \mu + \hbar\omega_c]$, where μ and ω_c are parameters of the model–μ needs not be equal to the chemical potential of the system, denoted here by μ_R. The BCS results are recovered if $\mu = \mu_R$. If $\mu \neq \mu_R$, the physical properties change significantly: the energy gap Δ is smaller than the BCS gap (see Fig. 4), a population imbalance appears (Fig. 5), and the superconductor-normal metal phase transition is of the first order (also Fig. 4). The quasiparticle imbalance is an equilibrium property that appears due to the asymmetry with respect to μ_R of the single-particle energy interval in which the pairing potential is manifested.

For $\mu_R - \mu$ taking values in some ranges, the equation for Δ may have more than one solution at the same temperature, forming branches of solutions when Δ is plotted vs $\mu_R - \mu$ at fixed T. The solution with the highest energy gap, which corresponds to the BCS solution when

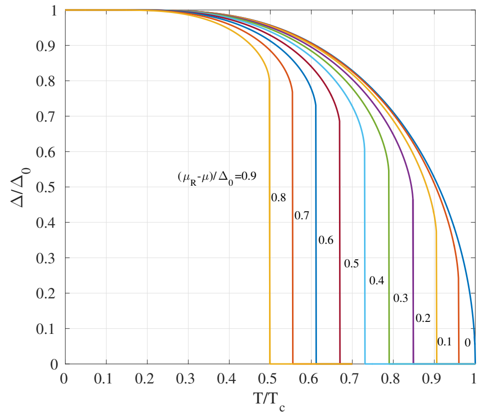

Figure 4: (The solutions for the energy gap Δ, for $(\mu_R - \mu)/\Delta_0 = 0, 0.1, \ldots, 0.9$; Δ_0 is the value of the gap energy at $T = 0$ and T_c is the BCS critical temperature (see Ref. [24]).

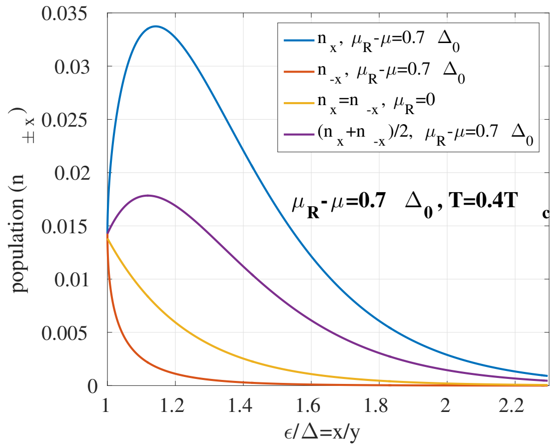

Figure 5: The branch imbalance, $n_x \neq n_{-x}$, for $\mu_R - \mu = 0.7\Delta_0$. For comparison we show also the typical BCS population, $n_x = n_{-x}$, for $\mu_R = \mu$, and the average $(n_x + n_{-x})/2$, for $\mu_R - \mu = 0.7\Delta_0$ (see Ref. [25]).

$\mu = \mu_R$, cease to exist if $|\mu - \mu_R| \geq 2\Delta_0$ (Δ_0 is the BCS gap at zero temperature). Therefore the superconductivity is conditioned by the existence of the pairing interaction and also by the value of $\mu_R - \mu$.

2 Further developments

We plan to continue the work of this project in at least two directions. We give here a brief description of our plan.

2.1 Dynamic and Thermal Properties of Micro- and Nanomechanical Structures

The currently developed technique of electronic microrefrigeration and nanothermometry usues the principle of "evacuation" of the electrons of higher energy from a metal via a normal metal-insulator-superconductor tunnel junction biased with a constant voltage. One of the main bottlenecks, limiting the refrigeration power of the electronic microcoolers (EMC) is the heat deposited and transported by phonons. Due to relative weakness of the electron-phonon interaction, electrons and phonons in the metal are almost thermally decoupled at sufficiently low temperatures. From our work during the project we note the similarities of the central element of these devices and the micro- and nanoelectromechanical resonators presently studied in different context and propose to investigate the thermal properties of these systems. Namely, the possibility of controlling the electron-phonon heat exchange via the electro-mechanical resonance driven by the a.c. biased tunneling. It is assumed this can enhance the electron-phonon heat exchange in the metal and thus would allow to effectively pump the heat out also from the crystal lattice. This new regime implies a deeper investigation of the normal vibrational modes and their coupling to electrons taking into account the composite structure of nanoelectromechanical resonators. In particular, it will not be possible to use the known solutions exploiting the symmetry of vibrational modes. We will derive explicit analytic form of the vibrational amplitudes required for the calculation of the electron-phonon matrix elements. Due to the specific geometry, based on our previous experience, the solution of the continuum elasticity equations will generate new waveguide modes (e.g., Stoneley) in addition to Rayleigh-Lamb waves. The electron-phonon coupling in metals is usually considered within the standard deformation potential approximation, but also the other mechanisms of coupling near resonance (e.g., parametric) will be considered. We shall also calculate the electron and phonon heat fluxes in this new (a.c.) regime and investigate their dependence on the parameters of the system to determine the optimized values. Overcoming the limitations of the presently used stationary tunneling current principle will enhance the electron-phonon heat transfer and, respectively, the cooling power of the EMC, which will give a new boost to the technology.

For the study of the effect of boundary and interface coupling on phonons from the perspective of quantum atomistic models we shall use our original method for solving the Schrödinger equation in discrete finite systems and calculation of quantum statistical averages. The advantage of this approach is that it allow to consider an arbitrary strength of coupling and finite temperatures and, in particular, will allow us to study the responsivity of a nanomechanical resonator of a cantilever geometry relevant for sensing devices.

An important future development of the project will be to consider propagation of heat driven by a periodic source which, as described above, generates thermal waves. This phenomenon constitutes the basis of the patent (A. Popescu et al., Non-invasive method and device for measurement of the thermal diffusion coefficient, Patent RO127565Bl, BOPI, nr. 8/2013) : the method and device for non-invasive and contactless measurement of the coefficient of thermal diffusion. The method uses the theory for thermal wave propagation developed for bulk materials. The used theory does not allow to obtain the correct description of the wave because at the microscale the behavior is even qualitatively modified (e.g., the Snell law for the heat waves breaks down). The non-invasive principle of measurement allows to meet the challenges of small size and power scales of the microdevices and is based on the dependence of the optical refractive index on temperature (exemplified, e.g., by the "mirage effect" in a desert). In contrast to the usual stationary heating of a spot of material (e.g. with a laser) and registering the temperature gradients which are necessarily rather high for a better resolution or a shorter thermal length. Instead, a low intensity laser beam is sent parallel to the surface. The heat wave (in our case generated by the a.c. current) periodically modulates the refractive index which in turn produces a modulated deviation of the beam. The phase shift of this modulation contains information on how the heat propagates both in the measured material and nearest environment. The latter in our case can be also the optically transparent silicon nitride. As we expect the signal to be weak, the focus will be on exploring the singularities in the wave propagation. Although the Snell law is not valid for thermal waves at short distances it is to be expected that the transmitted wave will have certain critical propagation directions dependent on the studied material. We will use alternative methods (e.g., Cagniard–de Hoop or Bellman-Marshak-Wing) to derive analytic expressions for the Green's function and calculate the corresponding phase shift angle for the probe laser beam. The novelty of this approach is that we will take into account the nanometric thickness of the the composite nanostructure, e.g., reflection and transmission of the thermal wave form the surfaces of the sample, which was not studied before. This can make the device for non-invasive measurement of thermal diffusion operational at the microscale.

2.2 Revision of the BCS theory of superconductivity and its applications

We shall continue the work started with Ref. [25], by investigating the new phenomenology that emerges from the BCS theory. We shall extend our study to unconventional and anisotropic superconductors and find applications to high temperature superconductors. After the publication of our paper [25], we found several experimental reports that need further interpretations and are in accordance with our findings (see for example Low Temp. Phys. **41**, 112, 2015; Phys. Rev. Lett. **87**, 047001, 2001; Phys. Rev. Lett., **87**, 137005, 2001; Science **314**, 1910, 2006; Phys. Rev. Lett. **98**, 267004, 2007).

3 Publications

3.1 ISI Journals

1. S. Cojocaru, Temperature dependence of magnetization of a nanosize Heisenberg ferromagnet, Opt. and Adv. Mat. Rap. Comm. 5, 1196 (2011).

2. D. V. Anghel, A.S. Parvan, A.S. Khvorostukhin, Fractional exclusion statistics applied to relativistic nuclear matter, Physica A 391, 2313 (2012).

3. D. V. Anghel, Fractional exclusion statistics – the method to describe interacting particle systems as ideal gases, Phys. Scr. 2012, 014079 (2012).

4. S. Cojocaru, L. A. Dohotaru, and V. A. Moskalenko, Shape anisotropy and magnetization of ferromagnetic nanostructures, J. Nano- and Optoelectronics 7, 719 (2012).

5. S. Cojocaru, Effect of boundary conditions on magnetization of a nano-size ferromagnet, Rom. Rep. Phys. 64, 1207 (2012).

6. G.A. Nemnes and S. Antohe, Spin filtering in graphene nanoribbons with Mn-doped boron nitride inclusions, Mater. Sci. Eng. B 178, 1347 (2013).

7. S. Cojocaru, Contrasting behavior of free-standing and embedded magnetic nanoparticles, Rom. Rep. Phys. 65, 832 (2013).

8. S. Cojocaru, L.A. Dohotaru, V.A. Moscalenco, Phenomenologic versus microscopic description of the nanoparticle magnetization, Rom. J. Phys. 58, 955 (2013).

9. G.A. Nemnes and C. Visan, Ab initio investigation of spin-filter effects in GaN nanowires with transitional metal impurities, Eur. Phys. J. Plus, **128**, 131 (2013).

10. G.A. Nemnes, Spin filtering effects in wurtzite and graphite-like AlN nanowires with Mn impurities, Journal of Nanomaterials 408475 (2013).

11. Dragos-Victor Anghel, George Alexandru Nemnes, Francesca Gulminelli, Equivalence between fractional exclusion statistics and self-consistent mean-field theory in interacting-particle systems in any number of dimensions, Phys. Rev. E 88, 042150 (2013).

12. D. V. Anghel and D. Churochkin, The anisotropic glassy properties of decagonal quasicrystals, Adv. Cond. Matt. Phys. 2013, 419202 (2013).

13. Dragos-Victor Anghel, From Fractional Exclusion Statistics Back to Bose and Fermi Distributions, Phys. Lett. A 377, 2922 (2013).

14. George Alexandru Nemnes and Dragos-Victor Anghel, Fractional exclusion statistics in non-homogeneous interacting particle systems, Rom. Rep. Phys. 66, 336 (2014).

15. S. Cojocaru, A. Naddeo and R. Citro, Modiffication of the Bloch Law in Ferromagnetic Nanostructures, EPL 106, 17001 (2014).

16. G. A. Nemnes and A. Nicolaev, Transport in ferrocene single molecules for terahertz applications, Phys. Chem. Chem. Phys. 16, 18478 (2014).

17. G. A. Nemnes and D. V. Anghel, Glassy behavior of disordered fractional exclusion statistics systems, Rom. J. Phys. 60, 691 (2015).

18. G. A. Nemnes and C. Visan, Electron transport properties of fulgide-based photochromic switches, RSC Advances 5, 26438 (2015).

19. G. A. Nemnes and C. Visan, Ab initio vibrational and thermal properties of carbon allotropes: polycyclic and rectangular networks, Comp. Mat. Sci. 109, 14 (2015).

20. A. E. Stanciu, G. A. Nemnes, and A. Manolescu, Thermoelectric effects in nanostructured quantum wires in the non-linear temperature regime, Rom. J. Phys. 60, 716 (2015).

21. A. A. Nila, G. A. Nemnes, and A. Manolescu, Ab initio investigation of optical properties in triangular graphene - boron nitride core-shell nanostructures, Rom. J. Phys. 60, 697 (2015).

22. D. V. Anghel and S. Cojocaru, Electron-phonon heat exchange in layered nano-systems, Solid State Communications 227 56 (2016) (arXiv1508.05184).

23. S. Cojocaru and D. V. Anghel, Low-temperature electron-phonon heat transfer in suspended metal films, Physical Review B, 93, 115405 (2016).

24. D.V. Anghel and G. A. Nemnes, The application of the fractional exclusion statistics to the BCS theory–a redefinition of the quasiparticle energies, Physica A 458, 276 (2016).

25. D.V. Anghel and G. A. Nemnes, The role of the chemical potential in the BCS theory, Physica A 464, 74 (2016).

3.2 Conference Proceedings

1. S. Cojocaru, Phenomenologic versus microscopic description of the nanoparticle magnetization, Proc. of the MSCMP, Chisinau, R. Moldova, ISBN: 978-9975-66-290-6, p. 38 (2012).

2. D. V. Anghel, Universal features in the thermodynamics and heat transport by particles of any statistics, J. Phys.: Conf. Ser. 338, 012002 (2012).

3. S. Cojocaru, L. Dohotaru, and V. Moscalenco, The Effect of Size, Shape and Environment on Magnetic Properties of a Nanoparticle: Microscopic Model Analysis; Proc. ICNBME-2013; International Conference on Nanotechnologies and Biomedical Engineering, ed. S. Raylean, (ASM, Chisinau) ISBN: 978-9975-62-343-8, pp. 322-325, (2013).

4. Dragos-Victor Anghel, Fractional exclusion statistics: the concept and some applications, J. Phys.: Conf. Ser. 410, 012121 (2013).

5. G.A. Nemnes and D.V. Anghel, Fractional exclusion statistics in systems with localized states, J. Phys.: Conf. Series 410, 012120 (2013).

6. S. Cojocaru and D. V. Anghel, Transfer of Heat Between Electrons and Phonons in Metallic Nanostructures, International Federation for Medical and Biological Engineering Proceedings Series 55, 21 (2015), ISBN: 978-981-287-735-2 (print) 978-981-287-736-9 (online).

7. D. V. Anghel, The stumbling block of the Gibbs entropy: the reality of the negative absolute temperatures, to appear in EPJ Web of Conferences 108, 02007 (2016).

8. Visan Camelia and G. A. Nemnes, Ab Initio Investigations of Thermoelectric Effects in Graphene - Boron Nitride Nanoribbons, EPJ Web of Conferences 108, 02045 (2016).

9. G. A. Nemnes and D. V. Anghel, A drift-diffusion model based on the fractional exclusion statistics, J. Phys.: Conf. Series 738, 012006 (2016).

3.3 Books

1. Eds.D. S. Delion, D. V. Anghel, I. Ghiu, and G. S. Paraoanu, Advanced many-body and statistical methods in mesoscopic systems II (Rom. J. Phys. 60, numbers 5-6, 2015).
2. Eds. D. V. Anghel, D. S. Delion and G. S. Paraoanu, Advanced many-body and statistical methods in mesoscopic systems (J. Phys.: Conf. Ser. 338, 011001, 2012, doi:10.1088/1742-6596/338/1/011001).

3.4 Conference organization

D. V. Anghel was one of the directors of the conference *Advanced many-body and statistical methods in mesoscopic systems II*, September, 1-5, 2014, Brasov, Romania.

3.5 Presentations in international conferences (made by the project members)

3.5.1 Invited

1. **S. Cojocaru**, Temperature dependence of magnetization of a nanosize Heisenberg ferromagnet, Opt. and Adv. Mat. – Rap. Comm. 5, 1196 (2011) (Invited talk).
2. **S. Cojocaru**, Phenomenologic versus microscopic description of the nanoparticle magnetization, 6th International Conference on Material Science and Condensed Matter Physics, September 11-14, Chisinau, Moldova, 2012 (Invited talk).
3. **D. V. Anghel**, Fractional exclusion statistics: the concept and some applications, International Conference on Mathematical Modeling in Physical Science, Budapest, Hungary, 2.09-8.09.2012 (Invited talk).
4. **G. A. Nemnes**, Fractional exclusion statistics in disordered interacting systems, International Conference on Mathematical Modeling in Physical Science, Budapest, Hungary, 2.09-8.09.2012 (Invited talk).
5. **S. Cojocaru** and V. Moscalenco, The Effect of Size, Shape and Environment on Magnetic Properties of a Nanoparticle: microscopic model analysis, 2nd International Conference on Nanotechnologies and Biomedical Engineering, Chisinau, Republic of Moldova, April 18-20, 2013 (Invited talk).
6. **D. V. Anghel**, Fractional exclusion statistics – the method to describe interacting particle systems as ideal gases, Frontiers of Quantum and Mesoscopic Thermodynamics, 29 July - 3 August 2013, Prague, Czech Republic (Invited talk).
7. **S. Cojocaru**, Some Mechanisms Relevant For The Control Of Magnetization In Ferromagnetic Nanoparticles, 7th International Conference on Materials Science and Condensed Matter Physics (MSCMP 2014), 16–19 September 2014, Chisinau, R.Moldova, (Invited talk).
8. **D. V. Anghel**, An introduction to fractional exclusion statistics: thermodynamics and transport, Complex and Magnetic Soft Matter Systems: Physico-Mechanical Properties and Structure (CMSMS 14), 29.09-3.10.2014, Dubna, Russia, (Invited lecture).

9. **S. Cojocaru** and D. V. Anghel, Transfer of Heat Between Electrons and Phonons in Metallic Nanostructures, 3rd International Conference on Nanotechnologies and Biomedical Engineering (ICNBME-2015), September 23-26, Chisinau, Moldova, 2015 (Invited talk).

10. **S. Cojocaru**, A generalization of the Bloch law for the temperature dependent magnetization of ferromagnetic nanoparticles, Advances in Nanophysics and Nanophotonics, 31.08-2.09.2015, Magurele, Romania (Invited talk).

11. **D. V. Anghel** and G. A. Nemnes, The BCS theory in the fractional exclusion statistics formalism, Frontiers of Quantum and Mesoscopic Thermodynamics, 27 July - 1 August 2015, Prague, Czech Republic (Invited talk).

12. **D. V. Anghel** and S. Cojocaru, Electron-phonon heat exchange in the layered structure of nanodetectors, Advances in Nanophysics and Nanophotonics, 31.08-2.09.2015, Magurele, Romania (Invited talk).

13. **S. Cojocaru**, Electron-Phonon Coupling and Heat Transfer in Layered Nanostructures at Low Temperatures, 4th Annual International Conference on Physics, 18-21 July 2016, Athens, Greece, p.12 (2016) (Invited talk).

14. **S. Cojocaru**, Electron-Phonon Coupling In Layered Nanostructures at Low Temperatures, 8th International Conference On Materials Science and Condensed Matter Physics September 12-16, 2016, Chisinau, Moldova, 2016 (Invited talk).

3.5.2 Oral and poster presentations

1. **D. V. Anghel** and D. Churochkin, Amended tunneling model to explain the anisotropy of the glassy properties of crystals and quasicrystals, APS March Meeting 2012, Boston, Massachusetts (poster).

2. **D. V. Anghel**, Fractional exclusion statistics: the paradigm to describe interacting particle systems, APS March Meeting 2012, Boston, Massachusetts (oral).

3. **D. V. Anghel**, Fractional exclusion statistics – the paradigm for the description of systems of interacting particles 9-14.07.2012: Dubna - Nano2012 Conference (poster).

4. **D. V. Anghel**, The anisotropy of the glassy properties of crystals and quasicrystals explained in an amended tunneling model (poster).

5. **D. V. Anghel**, Fractional exclusion statistics versus Fermi liquid theory a paradigm shift, 3-27.07.2012: International Conference on Nanoscience + Technology (ICN+T2012) (poster).

6. **D. V. Anghel**, I. M. Dumitru, A. G. Nemnes, D. V. Churuchkin, Models of two-levels systems for anisotropic glassy materials,APS March Meeting 2013, Baltimore, USA, 18-22.03.2013 (Oral).

7. **G.A. Nemnes** and D.V Anghel, Modeling of nanoscale transport using fractional exclusion statistics, APS March Meeting 2013, Baltimore, USA, 18-22.03.2013 (poster).

8. **D. V. Anghel**, Amended tunneling model for mesoscopic systems and anisotropic solids, MRS Spring Meeting, 1-5.04.2013 (Poster).

9. **D. V. Anghel**, Universal heat conductance in any number of dimensions, MRS Spring Meeting, 1-5.04.2013 (Oral).

10. **G. A. Nemnes** and D. V. Anghel, Modeling of nanoscale transport using fractional exclusion statistics, MRS Spring Meeting 2013, San Francisco, USA, 1-5.2013 (poster).

11. **D. V. Anghel**, Fractional exclusion statistics–perfection is in the eye of the beholder, New Trends in the Research of Carbon Based Nanomaterials, September 22-25, 2013, Magurele, Jud. Ilfov, Romania (oral).

12. **D. V. Anghel**, An introduction to fractional exclusion statistics: how to transform general interacting particle systems into ideal gases, TIM-13, 21-24.11.2013, Timisoara, Romania (oral).

13. **S. Cojocaru**, A Micrscopic Description Of Surface, Size And Shape Effects On Magnetic Properties Of Nanoparticles And Nanoclusters, Advanced many-body and statistical methods in mesoscopic systems II, September 1 - 5, 2014, Brasov, Romania (invited talk).

14. **D. V. Anghel**, Thermal properties of nanoscopic detectors, IBWAP 2014, 2-4.07.2014, (Poster).

15. **G. A. Nemnes**, Monte Carlo simulations for transport modeling using fractional exclusion statistics, IBWAP 2014, 2-4.07.2014, (Oral).

16. **G. A. Nemnes**, Monte Carlo approach to fractional exclusion statistics and applications, Advanced many-body and statistical methods in mesoscopic systems II, September 1 - 5, 2014, Brasov, Romania (oral).

17. **G. A. Nemnes** and C. Visan, Ab initio investigations of spin transport and thermoelectric effects in graphene - boron nitride nanoribbons, Mathematical Modeling and Computational Physics 2015, 13-17.07.2015, Stara Lesna, Slovacia (Oral).

18. **D. V. Anghel**, Gibbs vs Boltzmann statistics and the controversy about negative temperatures, Mathematical Modeling and Computational Physics 2015, 13-17.07.2015, Stara Lesna, Slovacia (Oral).

19. **G. A. Nemnes** and D. V. Anghel, A drift-diffusion model based on the fractional exclusion statistics, International Conference on Mathematical Modeling in Physical Sciences, IC-MSQUARE 2016, Athens, 23 - 27 May 2016 (oral).

20. **G. A. Nemnes**, Camelia Visan, D. V. Anghel and A. Manolescu, Molecular dynamics of halogenated graphene - hexagonal boron nitride nanoribbons, International Conference on Mathematical Modeling in Physical Sciences, IC-MSQUARE 2016, Athens, 23 - 27 May 2016 (Poster).

21. **D. V. Anghel**, The Application of the Fractional Exclusion Statistics to the BCS Theorya Redefinition of the Quasiparticle Energies, 5th International Conference on Superconductivity and Magnetism, 24-30.04.2016, Fethiye, Turkey (Oral).

22. **D. V. Anghel** and S. Cojocaru, Electron-phonon heat exchange in layered nanostructures, 18th International Conference MATERIALS, METHODS & TECHNOLOGIES, 2630 June 2016, Elenite, Bulgaria (Oral).

23. **D. V. Anghel** and S. Cojocaru, ELECTRON-PHONON INTERACTION IN NANOSTRUCTURES AT SUB-KELVIN TEMPERATURES, 16th INTERNATIONAL BALKAN WORKSHOP on APPLIED PHYSICS, 7-9.07.2016, Constanta, Romania (Oral).

3.6 Lectures in other universities and institutes

1. **D. V. Anghel**, A model for the dynamic defects in disordered materials, seminar at the BLTP JINR-Dubna, Russia.

2. **D. V. Anghel**, Fractional exclusion statistics vs. Fermi liquid theory – a paradigm shift, seminar at the University of Rhodes Island.

3. **D. V. Anghel**, Fractional exclusion statistics vs. Fermi liquid theory - a paradigm shift, seminar at the BLTP JINR-Dubna, Russia.

4. **D. V. Anghel**, Seminar Fractional Exclusion Statistics for Interacting Particle Systems, Laboratoire de Physique Corpusculaire de CAEN, 2-5.07.2012.

5. **D. V. Anghel**, Fractional exclusion statistics – concept and applications, Nanoscience Center, University of Jyväskylä, Finland, 19.08-1.09.2012.

6. **D. V. Anghel**, Fractional exclusion statistics – concept and applications, Seminar at the Aalto University, O. V. Luonasmaa Lab.

7. **D. V. Anghel**, Systems of interacting particles described as ideal gases with fractional exclusion statistics, 29.03.2013.

8. **D. V. Anghel**, five lectures on the physiscs of nanoscopic systems at the Summer School for MSc and PhD students: Hydrogen, Renewable Energy, Nanotechnology Applilcations, Ferdowsi University, Mashhad, Iran 17-19.06.2014.

4 Summary

During this project we addressed all the problems mentioned in the initial proposal and we adjusted our investigations according to the results obtained and the financial support provided. We published **25 papers in ISI journals with impact factor** (IF), **9 conference proceedings papers**, also in ISI indexed journals (without IF), we had **14 invited talks** in prestigious international conferences, and we made **23 contributed presentations** in international conferences.

In addition to this, we contributed to the organization of one international conference on the project's topic (DVA was one of the directors), we published two volumes of conference papers (also on the project's topic), and we gave 8 invited lectures in prestigious universities and research centers abroad.

In conclusion, we consider that the project's objectives have been achieved.