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PROJECT PROPOSAL
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Theoretical Research in Condensed Matter Physics.
Studies on Electronic, Atomic and Structural Correlations, Statistical Mechanics, Many-Body Theories and Quantum Effects of the Microscopic Interactions
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M. Apostol
Department of Theoretical Physics,
Institute of Atomic Physics, Magurele-Bucharest MG-6,
POBox MG-35, Romania
e-mail: apoma@theor1.ifa.ro

1 General Aim of the Proposal. Short Overview of the Field

The project is aimed at investigating the nature of the physical processes at the level of the condensed matter by theoretical physics methods. Its goal is to deepen our understanding of the condensed matter behaviour in various physical contexts, and to enlarge the modern scientific advances in the field, according to the current scientific research carried on nowadays all over the world in solid-state physics, materials physics, quantum gases and liquids, atomic and molecular structures, chemical systems, micro- and mesoscopic structures, quantum correlations, mathematical models of magnetic systems, disorder phenomena, etc.

Research in condensed matter physics is conducted nowadays all over the world in scientific research institutes, universities, and other research organizations, with an impressive vigour. Judging by the amount of scientific publications and the output of potential technological applications, the condensed matter physics rates by far among the most productive fields of research in modern physics. The reasons for this tremendous activity of scientific research are the internal wealth of fruitful problems of the field, its capacity of interpenetrating other fields of research (including, for instance, chemistry, biology, engineering, social sciences; therefore its multidisciplinarity potential), the huge capability of attracting a large labor force of scientific researchers, the comparatively small costs of research, and the potential technological applications that affect most directly the entire human society. From the total amount of Nobel prizes awarded in physics in the second half of the 20th century more than 70% went to condensed matter physics and related fields. It is worth mentioning here the 1996 Nobel prize in physics for the quantum liquid He3, and 1996 Nobel prize in chemistry for fullerenes, this latter domain enjoying, however, the highest curent activity in condensed matter physics. It is also worth mentioning the impressive technological applications and high-tech experimental techniques whereupon the condensed matter physics imprinted its indelible mark: silicon microelectronics, nuclear reactor materials, the laser, electronic and nuclear magnetic resonance techniques, medical imaging, the electronic microscope,

low-temperature physics and cryogeny, magnetic memories, molecular epitaxy, high-temperature superconductivity, etc.

In Romania the scientific research in condensed matter physics started around 1958, and, at least on the theoretical side, it was mainly conducted in the Department of Theoretical Physics of the Institute of Atomic Physics at Magurele-Bucharest. Though never enjoyed but a rather scarce funding, it was steadily growing up, and recorded notable achievemets in many-body theories of magnetic materials, phase transitions, electronic and structural processes in restricted geometries. In 70s and 80s the research field expanded considerably in this Department, both in widening its scope, enhancing the degree of mathematical rigour, and developing powerful techniques for treating a multitude of problems arising in the modern research, in conjunction with the most notable discoveries in the field. It is worth remarking in this respect that almost every big advance made in condensed matter physics in the world, and almost every notable modern trend in the field, has been illustrated over the years by original research carried out in the Department of Theoretical Physics. Out of but a short enumeration are the layered electronic materials (like graphite), quasi-one dimensional conductors, quantum gases and liquids, high-temperature superconductivity, fullerenes, electrons in magnetic field, microstructures, field-theoretical methods, renormalization group, path-integral methods, non-linear equations, strong electronic correlations, etc. The only notable areas of research which has not yet been covered are probably the amorphous semiconductors and large-scale numerical simulations; but, under a suitable conditioning, it is our intent to enter these research domains too, on a long-term perspective basis. It is however worth emphasizing that the scientific research in theoretical condensed matter physics in this Department has not only limited itself to its own field, but developed fruitful collaborations over the years with the scientific research in nuclear physics (four-fermion correlations in atomic nuclei), biophysics (configurational transitions in biomolecules), chemical physics (fullerenes and atomic clusters in solid-state matrices), materials physics (high-temperature superconductivity), mathematical physics (quantum liquids, superfluidity), general physics (transport phenomena, wave propagation), etc, both locally and in various other centres of research from abroad.

The scientific research in theoretical condensed matter physics is currently carried on in the world in the following main directions: fullerenes, high-temperature superconductivity, electronic correlations, quantum gases and liquids, electrons in magnetic field, atomic and molecular micro- and meso-structures, non-linear phenomena, chaotical and turbulent behaviour, low-dimensional solids, phase transitions, complex molecular systems, magnetic correlations, transport processes, defects, disordered and modulated phases, quasi-regular structures, wave propagation in non-regular geometries, quantum correlations, non-equilibrium processes, quasi-classical behaviour of complex quantum systems. The main problems in almost every one of these directions are very briefly outlined below.

In fullerenes research the mechanisms of attaching various chemical subunits to the main fullerene molecule is of utmost importance at this moment, in view of the alleged use of the fullerene molecules as physical vectors of active pharmaceutical principles; in this context, the endohedral fullerene molecules play a particular role. On the other hand, the peculiar structural behaviour of the solid-state fullerenes and alkali-doped fullerenes focuses the attention of the researchers in the field, together with the structural-electronic interplay in this compounds; among others, this is doubtless motivated by the rather high transition temperature toward a superconducting state, exhibited by these phases. It is noteworthy here the rather extended studies performed on fullerenes by our group.

In the high-temperature superconductivity continues the quest for the underlying mechanism of superconductivity in the cupprate oxides, and the relevance, from this point of view, of the

electron-lattice interactions and magnetic correlations. We note that an original mechanism of high-temperature superconductivity has been proposed within our reserach group even from the very beginning of this field. The theoretical research in this direction is however rather hampered by the lack of a local active research on the experimental side.
Related to this direction, the effects of the strong electronic correlations and the connected magnetic properties are under a very active scrutiny all over the world, with the hope of shedding light on the peculiar, strange enough, (often termed "abnormal") normal-state properties of the high-temperature superconducting materials. Though not in the least, the interest of the scientific researchers is also aroused in this direction by the electronic processes in the quasi-one-dimensional materials, especially the molecular and organic solids; speaking not of the very large, and active area of research in heavi-fermion systems. The Hubbard model and its various versions play here the main part, as the most studied mathematical model, and hopefully the most relevant, for the strong electronic correlations. We note here that starting with 1993 notable advances have been achieved by our research group in studying the Hubbard model in one dimension in a very original way.

Various instabilities and contrastant behaviour observed over the time in low-dimensional systems of interacting quantum particles led to new concepts of quantum liquids in contrast to the classical Fermi liquid. Various mathematical techniques, like bosonization, renormalization-group perturbation methods, field-theoretical methods, exact-solution methods, numerical computations, and even quasi-phenomenological analysis, pointed out new, distinct concepts like Luttinger liquid, marginal-Fermi liquid, abnormal, or, simply, non-normal Fermi liquid, etc. The main problem in this direction is the identification of a unitary framework, and the relationship between various model assumptions and predictions, such as to get a reliable understanding of one of the most basic problems in the condensed matter physics: the effects of the many-particle interactions, or many-body theories. We note in this context that various many-body techniques have been developed by our research group, among which, perhaps the most notable is the fermion bosonization in one dimension.

Electrons in magnetic field are studied in connection with the quantum Hall effect. There are two distinct ways of approaching the problem, as depending on the particular experimental setup. First, in an artificial, man-made, fabricated, MOS-type structure of a suitably small size, whereon an intense magnetic field is applied, such as to get what is called an "anti-dot" system; the electronic edge states that appears are thought as building up a chiral Luttinger liquid, and its transport phenomena are to be investigated with modern field-theoretical tools like the Chern-Simons-type theories. Secondly, natural solid-state compounds like the Bechgaard salts seem to provide another alternative for studying the problem; in this latter case, however, the quantum Hall effect seems to be associated with another subtle phenomenon, namely the field-induced spin-density wave. This occurrence is widely regarded as a special opportunity of exercising virtuosity in theoretical solid-state physics, in order to disentangle the two delicate processes. We note that original studies have recently been made by our group on the field-induced spin-density waves in Bechgaard salts.

Atomic clusters, fabricated nanostructures (like surface gratings, or multilayered structures), as well as regular, or quasi-regular atomic and molecular aggregates in solid-state matrices, carbon nanowires or amorphous silicon, provide a wealth of very interesting phenomena; they are extensively studied at this moment, both for their own scientific potential and for their technological applications. There are two main problems here. First, we must understand the way these structures form, why and under what circumstances they are stable, at equilibrium, and to what extent; secondly, the electronic levels of energy are pretty much inter-spaced as a consequence

of the finite-size effects, and we must adapt the (only available) solid-state theoretical methods devised for continuous energy spectra to this new situation. It is worth mentioning here that alkali clusters in ternary phases of alkali-doped fullerenes, as well as off-center sites in these compounds, have been extensively studied by our group; and recently we made some attempts toward the photoluminiscence of the amorphous silicon, in collaboration with experimental research conducted at Magurele.

Non-linear equations pervade today almost all the research areas in physics: non-linear waves, solitons, wave propagation in non-linear bodies, Thomas-Fermi equation, density-functional theory, non-linear master equations, etc, are relevant in classical physics, elasticity, physics of fluids, field theories, physical kinetics, and, obviously, in condensed matter physics; moreover, many applications of the methods lend by statistical physics and solid-state physics to biological, social, environmental, financial, political, informational and computing-related phenomena involve non-linear equations. Solitons associated with zero-sound excitations in one dimension, Thomas-Fermi equations for certain atomic clusters, interactive diffusion of two fluids, evolution of social conflicts have recently been treated by our research group by means of non-linear equations.

Complex systems with many degrees of freedom, usually non-linearly coupled, may exhibit a chaotical and turbulent behaviour. The main problems here are to assess the validity of the truncated model equations, to find out the generic degrees of freedom that describe the overall behaviour of the system, to search for the regular behaviour in chaotical temporal-series, to get the statistical description of the fluctuating, unstable, velocity increments. Concepts like universality classes, scaling, self-similarity, Lyapunov exponents, Poincare maps, phase-space trajectories, are employed to deal with such fascinating reserach problems.

Low dimensional solids, namely two-dimensional, layered and quasi-one-dimensional materials, and the associated theoretical models, are, very likely, the single leit-motiv of the scientific research in condensed matter physics in the 2nd half of the 20th century. It is worth mentioning here that this area of research has always been illustrated very well by the activity of our group. Here there is a multitude of very interesting phenomena and problems. In two dimensional and layered structures one has to further clarify the role of the nested Femi surface and the alleged deviations from a Fermi liquid behaviour. In one dimensional systems it remains to get a firm basis for understanding the effects of interactions, especially between electrons. The role of the quantum fluctuations in low dimensions is still amenable to a deeper grasp.

Phase transitions are one of the most topical investigations in condensed matter physics. Structural, electronic, magnetic, ferroelectric transitions, Bose-Einstein condensation, superfluidity, superconductivity, charge- and spin-density waves, etc, are but a few examples. The main problems today in this area are the role of the fluctuations, the effect of the dimensionality, the part played by disorder, the response to external probes, and the dynamics of the order parameter near a critical point. Of particular interest here are the disordered lattice systems and the associated continuous spin models. Most of these problems are under current investigations in our group.

Copper-oxygen octahedra and pyramids in high-temperature superconducting materials, quasi-spherical fullerene molecule made of 60 carbon atoms, endohedral fullerene molecules, atomic clusters with regular or irregular geometries, hexagonal and pentagonal sheets of carbon atoms, complex ligands in molecular and organic solids, etc, are examples of complex molecular systems. They are tractable in principle by a combination of theoretical tools borrowed from atomic, molecular, solid-state, statistical physics and physical chemistry. This is almost a unique situation, where so many different methods are put together for getting an insight into such complex

systems. The main problem here is to critically analyze the validity range of each of the above-mentioned methods, try to extend them to these new situations, and be able to interpret the output correctly, i.e. in agreement with the general principles of theoretical physics. Research in this area is also illustrated by the activity of our group, as, for instance, our original research in the Thomas-Fermi theory of atomic clusters, NMR spectra of alkali-doped fullerides, fullerene anion, etc.

Antiferomagnetic fluctuations at low doping level in cupprate oxides, abnormal magnetic susceptibilities in heavy-fermion systems, magnetic response of the spin- and structural-modulated phases, as well as the recent reports on giant magnetoresistance materials imply strong magnetic correlations. The problem here is to establish the connection between these magnetic properties and the associated structural and electronic processes, and to further ellaborate upon the existing magnetic models as to incorporate these new features. It is worth emphasizing here that our research group has a highly rated expertise in magnetic models like the spherical Ising models, or random field models of statistical physics.

Extensive studies are currently performed at this moment on the thermal and electrical conductivities of various compounds, and on various fabricated solid-state structures. The main problems here are, on one hand, to adapt the classical theories of transport phenomena, devised, mainly, for homogeneous, infinite physical systems, to newly discovered materials which exhibit deviations from these uniformities, and, on the other hand, to decipher strange transport processes, like ballistic transport, coherent tunneling at the superconductor-normal metal junctions, finite size effects, etc. Mass transport, thermoconductivity, electrical conductivity , thermopower, and order parameter transport have been extensively studied in our group, though, perhaps, not very impressivelly illustrated at the level of the scientific publications.

Defects are everywhere in realistic condensed matter; nothing is perfect in our natuarl world, and we have to accommodate them in our ideal mathematical models, and to allow for their important effects. Impurities, vacancies, substitutions, quasi-modulated phases, domain walls, fractures, vortices, random fields, fluctuations, frustrations, have their own dynamics, i.e. move, interact, superpose to each others, interfere, and may drastically affect the behaviour of the main process. The main problem here is precisely the study of this defect dynamics, and its consequences. Off-centre sites in homogeneous phases, the role played by the vacancy dynamics in the NMR spectra, the defects thermodynamics at very low temperature have been studied recently by our group. Disordered and modulated phases represent another aspect of the defect dynamics, in the sense that the former is, generally, tractable with the tools of the statistical mecahnics, while the other represent hierarchical perturbations superimposed over regular phases. Generally, the extent of the symmetry breaking is brought into discussion here, and how certain lower long-range orders develop from other higher long-range orders.

Quasi-regular structures have been identified over the time in condensed matter physics, and they are not only a subject of awe, but one of pragmatic, mathematically exact, scientific investigation. Aperiodic crystals, quasi-regular backbones of the huge biomolecules, Langmuir films and liquid crystals, quasicrystals of rather common alloys, and, finally, all-over-pervading fractals, are examples of such structures. Almost any meaningful question in the field of theoretical physics remains largely unanswered as regards these structures. The deep connection between the geometry, dimensionality and the physical processes is the main problem in this area of research.

Wave propagation in non-regular geometries is a fascinating problem. Almost any motion in condensed matter may be analyzed in terms of waves. This means, however, that a presupposition

is made as regarding certain homogeneities, small responses, and regular geometrical properties of the physical system. The realistic situations we encounter so frequently are far from this ideal situation. Suppose that we have a rough line, or surface; what does a travelling wave look like, and what are its local effects? What are the global parameteres in terms of which we can characterize the propagation, reflection, transmision of such a wave? How the energy is dissipated in such a body with a rough geometry? In certain chemical reactions which take place in a condensed body wave fronts built up, that have a shape and propagate with a velocity. What is the relationship between the shape and the velocity of the wave front? Phase transitions do often take place behind a propagating wave front; what is the order of the phase transitionin such a process, having known that we only have a certain understanding of the phase transitions in infinite, homogeneous media? What are the local effects of a seismic wave on the earth surface, where there are so many inhomogeneities, and such a structured geometry? The latter being only an example of how practical such an investigation could be.

An overwhelming majority of striking macroscopic phenomena proceed at the level of the condensed matter purely on the basis of quantum correlations. Helium superfluidity and superconductivity are the most typical examples. The latter is known to arise from the fermion statistics and certain interference effects of the wave-like nature of the electrons; the former, however, while implying the same wave-like nature of the boson particles, seems to avoid the interference effects, and precisely in this avoiding resides another special type of quantum correlations; because both phenomena are the most typical examples of quantum correlations, and the macroscopic quantum wavefunctions. Quantum particles our world is made of possess "hiden" particularities as regards their availability of the entire phase space, and the deep cause of these correlations remains largely unknown. The main problem here is to test the manifestation of these quantum correlations in various physical contexts, as, for example, various dimensions, magnetic fields, restricted geometries, etc, with the hope of deepening the quantum nature of our macroscopic world. Studies on Bose-Einstein condensation, superfluidity, dimensionality effects on the quantum phases, have continuously been pursued by our research group.

Non-equilibrium processes are extensively studied at this moment, due to the large variety of complex behaviour they involve, on one hand, and, on the other, due to their ubiquity in condensed matter systems. Physical kinetics provide the general frame of treating the approach to equilibrium at long times and over long distances; the main problem here is to incorporate in such theories the behaviour over short spatio-temporal scales. This implies both higher order differential equations and non-linear contributions, correlations, fluctuations, feedback, memory functions and history-dependent processes.

Finally, quasi-classical behaviour of complex quantum systems is a problem raised by numerous experimental observations which pointed out that complex many-body systems of interacting quantum particles often exhibit a quasi-classical behaviour; hydrodynamic approaches, mean-field theories, path-integral formalisms, etc, try to capture this specific behaviour. Contrary to what is commonly believed, such approaches do not leave aside the essentially quantum nature of these systems, but are aimed at including precisely those underlying quantum structures and mathematical concepts that are essential for the observed behaviour.

2 Recent Local Achievements (1992 -)

Our research group of theoretical condensed matter physics has obtained many notable achievements during the time. They are recorded in cca 60 scientific papers, published abroad by 4

authors, and will be briefly reviewed below, with emphasis on the relevance these achievements bear upon the main areas of research in the field; at the same time, we note that most of these achievements are still under current study within our group, in a continuous effort of taking them to a further development.

In our group it has been developed for the first time an original model of a spherical molecule for treating the molecular vibrations, rotations and deformations of the fullerene molecule. It has been shown that, within this model, the fullerene molecule is stable, its rotations are decoupled from vibrations to a large extent, and new motion equations have been derived, and partly solved, for certain spherical vibrations of the molecular surface. The electrons moving about such a spherical molecule have also been studied, and energy spectra for the fullerene anion and dianion have been obtained in good agreement with the experimental data. Off-centre sites of the alkali cations in alkali-doped fullerides have been reported by us for the first time in the scientific literature, by studying the van der Waals interactions between the fullerene molecules in solid-state phase. A new effect has thereby been predicted on the assymetrical shape of the NMR spectrum of the alkali cations in the tetrahedral coordinations, which is currently studied by the experimentalists. The vacancy dynamics has also been studied in the ternary phases of the alkali-doped fullerides, and found that they may explain a strange feature in the NMR spectrum observed experimentally since a few years (the so-called T-T' splitting), and unexplained till now. A basic reconsideration of the defect formation in solid state has been prompted by such studies on fullerenes, thus contributing toward a deeper understanding of the basic phenomena in condensed matter physics. Under certain circumstances, related to the doping level, the alkali cations in the fullerene cages formed in these compounds organize themselves in atomic clusters of regular shapes, like, for instance, cubes, body-centered cubes, tetrahedra, etc. This is a subject of intensive study, both experimentally and theoretically, and we have formulated a theoretical approach to this problem, which is able to give consistent answers to various questions concerning the stability, the equilibrium, the degree of ionization, the interpaly between ionicity and other chemical bondings, etc. More general studies have been prompted by this problem, too, as regards, for instance the general Thomas-Fermi theories of atomic structures, chemical binding, complex molecular aggregates, etc. It is worth stressing here that, in spite of our rather modest means, we made a true theoretical breaktrough in the fullerene research area, which is deemed as one of the most competitive area in the current scientific research.

One of the most remarkable achievements of our group are the theoretical studies on the Hubbard model in one dimension, and its extended versions. These studies are carried out by a highly original method, recorded as such in the scientific literature. Specifically, the method consists in treating the interacting Hubbard gas as a fermion gas in the dilute limit by means of the Bruckner pair approximation. Surprisingly enough the method can be applied consistently to produce the ground-state energy, correlation functions, and even elementary excitations in one dimension. Phase diagrams of extended Hubbard models in one dimension has thereby been obtained as functions of density, and various types of instabilities have been pointed out. Moreover, these very interesting results, obtained, as it was said, within a typical perturbative approach, raise the question of the various relationships that may exist between the perturbation theories and some exact solutions available for these models. The models are relevant for the high-temperature superconducting materials, and for certain quasi-one-dimensional organic compounds, where the strong electron correlations are the main problem. Various interaction processes, like on-site, inter-site, intra-bond, inter-bond, bond-site interactions, etc, have been treatead thoroughly, and their effect for various densities have been elucidated. The Bruckner theory has been extended in our theoretical studies in a systematic way, such as to include the selfconsistencies of the electronic interaction processes, and, by now, it became a powerful tool of investigating systematically the

entire interaction phenomena in such a large variety as the quasi-one-dimensional Hubbard-type models. Our group has been able to establish many external collaborations in this area of research.

Another very remarkable achievement of our group consists in the theory of the off-centre diffusion and its application to the Oswald ripening process. First of all, the anomalously large diffusion coefficients of certain substitutional impurities in alkali halides have been related with the off-centre positions these impurities may acquire in the host lattice. It was for the first time in the scientific literature that they off-centre sites were shown to play the essential role in the impurity diffusion. Secondly, the phenomenological theory of diffusion was revisited, and new master equations have been derived starting from the elementary acts of the diffusional process. It was recognized that in the overwhelming experimental situations the long distances and the long times play the essential role in diffusion. These equations have thereafter been devised in such a manner as to include the off-centre sites which build themselves around the normal sites in certain star-patterns with various site numbers and various internal symmetries. The explicit solutions have been given to these equations by employing the classical Fourier analysis and the symmetry properties. It has been studied all the classes of cubic symmetry in one, two and three dimensions, and it may suffice to say, for instance, that in some cases the system of equations comprise more than 20, or 30, equations. It is worth mentioning that analytical solutions were given by the above-mentioned technique, and the solution with the lowest frequency was given everywhere a particular attention. A general perturbative method has also been developed for treating these off-centre equations for an arbitrrary symmetry. It has been discovered that an universal geometric factor affects all the diffusion coefficients, depending on the number of off-centre sites and their own symmetry with respect to the symmetry of the host lattice.
The method of this geometrical factor has then applied to a much studied phenomenon in the cluster physics, namely the Oswald ripening. We were able to reformulate the only exising theory of this phenomenon - the Lifshitz-Slezev theory - , to give its validity limits, and to extend it to the intermediate regimes of clustering. Indeed, it was shown that this classic theory is valid in the asymptotic limit of very long times and one huge cluster, where the clusterization goes like the third power of the time. Before this final stage of clustering, however, we have identified an intermediate stage where the temporal law is the sixth power of the time, in agreement with all the available experimental observations. We are, thereby, in possession of a powerful theory of treating the clusterization phenomena in those parameter regions where almost all the experiments are conducted and where no theoretical approach was available untill now.

Rigurous models of statistical physics have extensively been studied by our group with notable results. The phase diagram of the generalized spherical model of a random ferromagnet has been investigated from the paramagnetic region, and arguments have been given in favour of a Griffiths intermediate state. The Bogoliubov model of superfluidity has been shown to have stability problems, and its suitability for describing the superfluid transition, and the related Bose-Einstein condensation, has been questioned. A soft cutoff has been introduced in order to remove these inadequacies, whose consequences are still to be further investigated. The quantum mean-field state of a hot dense plasma has been derived as a limit of canonical states in a Wiener integral approach, allowing a better control of the Hartree equation and its classical limit. The occurrence of the nematic order has been established for a two-dimensional model with long-range interaction, and the corresponding critical behaviour has numerically been investigated.

Studies on one-dimensional many-fermion systems were continued in our group of research, and are of continuing interest. After having devised in the past the appropriate form of boson representation of the fermion fields in one dimension, and having explored its consequences on the interaction processes in quasi-one-dimensional systems, a more flexible version of bosonization

has been derived recently, by means of the quasi-classical approximation method. This bosonization allows one to understand the basic nature of the fermion-boson duality in one dimension, and it lends itself to various applications which were deemed as almost intractable untill now. The well-known Luttinger liquid has been rederived by means of this method, and it was also extended beyond the low-lying boson-like excitations by incorporating the interference effects of the right-moving and left-moving fermions. It has obtained in this way a new type of excitation in these systems, namely a soliton associated with the zero-sound type of processes occurring in a normal Fermi liquid. The well-known interaction processes in one dimension, classified by the "g-ology" theories in forward scattering, backward scattering and umklapp scattering, with and without fermion-branch and spin flip, are much more directly obtained in this formalism, and their various physical consequences are much easier to be assessed. Moreover, the formalism is very well adapted to treating more complex problems as the electron-phonon interaction in one dimension, or the inter-chain coupling, the physics of the coupled Luttinger, and beyond-Luttinger liquids, problems of large interest at this moment in the scientific community. The transport properties of these quantum liquids, especially the electric conduction, including superconductor-normal metal junctions are also tractable rather straightforwardly by the quasi-classical bosonization. It is worth stressing that this method, and the corresponding version of bosonization, is a notable advance in the theoretical studies of the non-Fermi quantum liquids.

Classical and quantum transport phenomena have been revisited, with emphasis on the finite life-time processes of elementary transport. The phonon thermoconductivity of a finite-size, ideal lattice has been derived, and, following the same method, the electric conductivity and thermopower have been studied, for various typical situations, like normal metals, semiconductors, quasi-one-dimensional compounds, etc. Applications have been made to recent experimental data on the thermoconductivity of some quasi-one-dimensional materials, whose both phonon spectrum and the electrical carries exhibit typically significant deviations from those of the ideal solid. At the same time, the connection has been made to the transport properties of the condensed phases, especially the superconducting and the charge-density-waves phases, near the critical point. The method has been applied also to a rather different type of process, the sound attenuation near a critical point, and a new, general mechanism of sound attenuation has been formulated in this case. It is based on the specific dynamics of the order parameter of the phase transition near the critical point, especially on the phase dynamics of this parameter. The mechanism has been applied to puzzling experimental data in quasi-one-dimensional compounds exhibiting transitions toward a charge-density-wave state, and a good agreement has been obtained, together with an understanding of the physical processes involved. Related to the dynamics of the order pararmeter it is worth mentioning that the thermoconductivity (as well as the specific heat) of the phase excitations have also been derived for the first time in the case of the charge-density waves. All this research has turned out to be of significant relevance for the physics of the quasi-one-dimensional materials, which is one of the most active fields of research at this moment.

A very interesting problem has recently been solved by our group, concerning the relationship between the magnetic field and the spin-density wave in Bechgaard salts. These compounds are of much interest because they may provide a natural system for the quantum Hall effect. However, the situation is a bit more complicated than in the usual, fabricated structures, since a spin-density wave accompanies the magnetic field. This transition has been observed by the thermodynamical parameters, and never directly observed by the in-plane modulated spin density as one naively would have expected. The existing theoretical approaches are usually making use of the assumption that these compounds are quasi-one-dimensional; which they are, structurally; but the careful analysis shows that electronically, and especially when the magnetic field is applied, they turn out to be effectively two-dimensional. In addition, the large electronic anisotropy of

these compounds make them to behave as two-dimensional quasi-free electronic systems in the effective-mass approximation. This is a very unusual situation, and it must be stressed that it is due entirely to a certain range of electronic and structural parameters, which fall in a very narrow window; and, it is quite amazing that these compounds are naturally tailored in precisely this manner, which makes their study very attractive, indeed. The whole theory of the electron motion in a magnetic field has had to be reconsidered for such anisotropic situations in order to identify quantitatively this special behaviour. This opens the way, on the other hand, to the investiagtion of the quantum Hall effect in these natural structures. It was predicted, beside all the observed thermodynamical quantities of this field induced spin-density wave, that the wavevector modulation of the spin density takes place almost perpendicular to the planes, instead of residing in the planes. This prediction is a matter of current pondering on behalf of the experimentalists.

Quantum and statistical correlations, brought about by the indiscernability of the quantum particles, have also been studied, especially in low-dimensional systems, for the collective modes of the normal many-particle systems, and in the condensed phases of the second-order phase transitions. It has been shown that a recent inequality involving the structure factor of the many-particle systems is nothing but another form of the definition of the structure factor and the effect of the the well-known sum rules. The method used for rederiving this inequality served to extend this inequality such as to incorporate the collective modes and the condensed modes of the order parameter. Explicit applications have been done for plasmons, for the zero-sound in the normal Fermi liquid, and for the Bose-Einstein condensation and generally for the superfluid transitions. This type of research aims to deepen our understanding of the basic features of the interacting many-particle systems, like the collective modes, the symmetry breaking, the off-diagonal long-range order, the macroscopic quantum wavefunction, etc. Another type of quantum correlations (and fluctuations) have been studied in connection with the low dimensional solids. It is well-known that these solids are unstable, both at zero and at finite temperatures, as a result of the atomic fluctuations in the harmonic approximation. It has been shown that these solids can be stabilized under these fluctuations by imposing certain constraints on their motion, in agreement with the actual experimental situation. More precisely, these constraints arise from the substrate these solids are always deposited on, and the consequences of these special conditions on the vibration spectra have been investigated. Besides stabilizing them by this device, it has also been shown that these solids have a finite temperature of melting. The latter was computed in the harmonical self-consistent approximation both for one-, two- and three-dimensional lattice, and the well-known Lindemann criterion of melting has thereby been obtained.

An original theory of high-tempertaure superconductivity has been developed by our group for the cupprate oxides. It is based on the local distortion of the copper-oxygen octahedra and pyramids, due to the displacive modes of the oxygen anions in these molecular complex. Basic experimental facts are included by this theory, like the lattice vibration spectrum, the charge carriers, the tilting modes of the octahedra and the "dimple" modes of the pyramids. At this stage the theory does not take into account the retardation of the pairing interaction, and the particular features of the Fermi sea; for instance, the change of the charge carriers from holes to electrons on increasing the doping level is left aside. However, the theory is able to predict the main experimental features of the phenomenon, like the dependence of the superconducting parameters on the hole concentration (i.e. the doping level), the anomalous isotope shifts, the relationship between the critical temperature and the tilting angle, etc, all these predictions being left to be further checked on experimentally.

3 Work in Progress

In the next six months the general theoretical framework will hopefully be established for getting a physical description of the ferroelectric transition in SmB6. A symmetry breaking has recently been reported in this compound involving the spatial inversion. This investigation falls into the class of the phase transition research, this time being discussed a comparatively rare case, namely the relationship between the rather localized f-electron states, of an atomic-like nature, and the more extended d-electron states, resembling more the conduction band states in normal, simple metals. The compound belongs to the transition-elements family, where little is actually known, despite of extensive investigations performed in the past on the magnetic, structural and conducting properties. The ferroelectric transition is usually associated with a corresponding structural transition, toward a state with a permanent, non-vanishing local electric moment (dipole). The possibility of a ferroelectric transition driven by the interaction between two electronic state partners is a new possibility, recently highlighted, whose nature is still far to be understood. The problem is in fact more complicate, as there is already a description of a similar transition as a first-order one, while many other experimental data seem to indicate a second-order transition. The difficulties related with having reliable data for the time being can hopefully be circumvented by a rigurous theoretical analysis, which will be able to give a clear-cut distinction between the properties of a first-order transition and a second-order one in this particular case. The basic ingredients of the theoretical models will be critically analyzed, as regards the various types of intercations between the two-bands electrons permited by the lattice symmetry and the general asssumptions of the tight-binding approximation. The ferroelectric state will be obtained by standard techniques, and its properties wil be investigated as functions of the various model parameters. In the next step the optical response will be investigated, which seems to be the main experimental tool of getting accurate information in this case. More general problems will be raised thereafter, as regards the type of order, the quantum correlations involved, general spin models that could be used more comfortably for treating similar problems. We emphasize that this is a completely new problem in the field of the condensed matter physics, which, however, lends itself to a conceptually known treatment, at least in principle. It is also worth emphasizing that the dynamics of the f- and d-electrons in trasitional elements has been given much attention in the past, and is still a matter of extensive research.

The work on the strongly correlated electrons in one-dimensional systems is another objective of our research group. On a short-term basis the Hubbard model with a bipartite lattice will be approached within the renormalization group method. This method has been devised in the past specifically for computing the critical exponents of the phase transitions; almost at the same time it has been extended to treating the various classes of equivalence of many-particle systems, by using the scaling concept. Among others, the method proved to be very valuable in the case of the one-dimensional systems, where the logarithmic singularities asociated with various interaction processes dictate the physical behaviour of the system. Writing down the main diagramatic contributions to the effective interactions, applying the renormalization procedures, and solving for the scaling equations, enables one to get a renormalization-group diagram for the effective coupling constants whereon various classes of equivalence can be read. Moreover, the singularities of the response functions can be obtained in this way, such that a phase diagram results, pointing out the possible phases of an interacting many-body system. In the case of the Hubbard model the interest resides in the change of the phase diagram on varying the filling factor, i.e. the electron density. It is known that a rather rich phase diagram is obtained for the classical version of the Hubbard model, suggesting thus a particularly correlated physics of the intercating fermions. For a bipartite lattice in one dimension the phase diagram is even richer, involving

singlet and triplet superconductivity, charge- and spin-density waves, modulated phases of the umklapp scattering processes, etc. It is worth noting that an extended version of the Hubbard model is studied in one dimension, i.e. one wherein not only the on-site interaction is taken into account, but also inter-site interactions, bond-site intercations, inter- and intr-bond interactions are included. The coupling constants of all these interaction processes depend themselves on the electron density, so that trough the renormalization-group equations this dependence is propagated into the phase diagram of the model. The two main classes of equivalence are obtained, namely the Luttinger-type liquids and the Luther-Emery-type exactly-soluble models. Critical exponents of the corresponding correlation functions are to be computed in the next stage of this research, and the very interesting inter-chain coupling problem remains to be tackled. By solving such type of problems one gets an insight of what type of physical behaviour a certain model might exhibit, in the sense of what equivalence class that model fall in; and secondly, one may assess whether the further pursuing of a given model is worth of. For instance, the bipartite Hubbard model in one dimension is thought to be relevant for the copper-oxygen chains in the highly superconducting cupprate oxides.

Theoretical research on fullerenes is running on. The main attention is given in the next future to the stability of the endohedral fullerene molecules. These are molecular aggregates made of a quasi-spherical fullerene molecule which may take inside an atom, or a group of atoms. The problem is to assess the stability of this system. The main method of approaching this problem is by means of the Thomas-Fermi theory. The system consists of a certain distribution of positive charges, displayed over a quasi-spherical surface, and another central point-like charge, plus the moving electrons obeying the Fermi statistics. If one approximates the fullerene molecule with a spherical shell the resulting molecular complex is unstable within the Thomas-Fermi theory. One is therefore forced to go beyond the spherical approximation, *i.e.* to take into account the discrete distribution of the carbon atoms on the molecular shell. However, this implies a refinement of the standard Thomas-Fermi theory, and the solution of the corresponding non-linear equation can only be obtained by numerical computation. Preliminary calculations show indeed that the system is stable now. The next step in this direction is to compute the normal modes of motion of the central atom or group of atoms, which would be a much sought result, as the corresponding frequencies can be tested experimentally in Raman scattering, electron energy loss spectroscopy, etc. The attachment of various other chemical subunits to the fullerene molecule is another point of interest in this research, contributing to the understanding of the physical and chemical properties of this complex molecular system. The high symmetry of the fullerene molecule, and the large number of atoms it consists of, provide the opportunity of treating this new molecular object by the standard techniques borrowed from statistical physics and solid-state physics. It is worth emphasizing here that this is almost a unique opportunity in the field of molecular physics, able to open unexpected theoretical ways in this scientific research. However, it must be stressed on the other hand, that the above mentioned methods have to be adapted to the quasi-spherical symmetry at hand, being known that they have originally been devised for infinite, homogeneous physical systems. A similar situation have already occurred in the physics of the layered and quasi-one-dimensional materials.

Related to this direction of research the investigation of complex biomolecular systems is also running on. These systems exhibit a complex dynamics, and the efforts are directed toward highlighting the overall behaviour relevant for the main, observable physical and chemical processes. The interaction between the receptors on the surface of the living cells and the surrounding growth factors is under current investigation. Non-linear diffusion seems to govern these processes, including a self-consistent, self-regulatory and feedback-controlled behaviour. The experience in off-centre diffusion is put at work in this direction of research.

Work on magnetic models, rigurous mathematical models of phase transitions, the role played by fluctuations in anharmonic crystals is in progress. The decay of two-spin correlation functions is investigated in the generalized spherical model. Two types of long-range behaviour are shown to exist for transverse and longitudinal correlations in this model, supporting the renormalization-group predictions. The theory of Bogoliubov for the superfluid transition is further studied, with emphasis on the role played by the cut-off on the excitation spectrum.

Quantum and statistical correlations are further on studied in quatum gases and liquids. First, the effects of the intercation are on the focus, in particular their manifestations in the two-particle processes. This is a problem which has not received a special, programatic attention in the past, though there were many signals that the two-particle correlations might play an unexpected role in our understanding of the interaction effects in many-particle physics. It is well-known that a large class of systems are described by their one-particle properties, as, for instance, the Fermi liquids; there are also various collective modes both in these systems and in the condensed ones; and, finally, there are systems whose essential behaviour is dictated by diagonal, or off-diagonal long-range order. Multi-particle correlations, and in particular the two-particle ones, promise to reveal new features in the quantum effects of the interacting systems. On the othe hand, the statistical correlations may reveal new sides in the physics of the quantum gases and liquids. Superfluidity, superconductivity, charge- ans spin-density waves exhibit unexpected features, especially in low dimensions. A certain equivalence, for example, has recently been reported between the Fermi and the Bose ideal gases in two dimensions, arising, apparently, from the boson-like correlations, responsible, in three dimensions, for the superfluidity phenomenon. By the same token, research is conducted in estimating the effect of fluctuations on certain non-linear statistical models approaching equilibrium. This research belongs to physical kinetics, statistical physics, and may lead to relevant results in other fields, as, for instance, social phenomena.

Another direction of research wherein current advances are made is the investigation of the underlying mathematical structure of the basic equations of mathematical physics in certain new physical contexts. As it is well-known, various fields of research in physics, condensed matter physics included, employ more or less similar mathematical tools, and, very often, new insights and powerful methods of investigation developed in one field turn out to be significant in another field. A large class of phenomena in condensed matter physics are described, for example, by the classical wave equation, or by Schrodinger equation. Similar equations appear also in describing the properties of the elastic media, or in describing traveling waves in certain constrained geometries. The effects of these phenomena on surfaces with non-uniformities, with defects, with angular points, on rough surfaces, etc, are of great interest, since these situations can also be encountered in solid-state physics. This is a new and very promising direction of research, wherein, hopefully, more significant advances are to be made in the future.

4 Long-term perspectives

The present research project has short-term (about 6 months), middle-term (cca 1 year) and long-term goals. The former two are outlined in the previous section. Their successful accomplishment is warranted by their own internal consistency, scientific soundness, and the experience our group acquired over the years in this field of research. Before turning to the long-term perspectives of the project, it is perhaps worth remarking that its main objectives and the specific goals place themselves along the main lines of research carried on at present in theoretical condensed matter physics in the world. The associated list of publications shows clearly that the research performed in our group meets the high standards of the scientific research in the most advanced countries.

The tremendous activity of scientific research in condensed matter physics will result in the coming few years in new and unexpected scientific discoveries in various directions of the field. The end of this millenium, and the beginning of the third, will witness new materials, new technological applications, new physical effects, new atomic and molecular structures, new experimental techniques and theoretical methods, all these as a consequence of the big financial and human-resource efforts that are being made. These achievements will provide a great challenge to the theorists for placing them in the general frames of the theoretical physics. While trying to keep abreast with the modern discoveries and the modern experimental techniques in the field, the physical research in Romania will also face the much lower costs of the associated theoretical research. The main output of the latter, however, ensures, on one hand, the necessary knowledge, *i.e.* the cheapest and, at the same time, the highest acquisition, - since it provides the understanding; in economical terms it may be viewed, therefore, as the most efficient activity in scietific research; and, on the other hand, it ensures the world representativity of Romanian scientists, by their publications, participation in the international scientific meetings, and external collaborations.

The fullerene research direction will record, undoubtedly, impressive advances toward complex molecular aggregates containing fullerenes; the stability of such structures, and their specific quantum dynamics is one of the long-term goal of the present project. High-temperature superconductivity will hopefully reach the basic understanding of the essential role played by the lattice dynamics, particularly by the local displacive modes of the oxygen atoms; which is also one of our long-term goal in this area of research, according to the previous experience of our group. On the other hand, the strong electron correlations will undoubtedly reveal the underlying quantum structures, and, in this context, our studies on the Hubard model and the related versions will help to clarify these matters. The multi-particle correlations, particularly the two-particle correlations, are also expected to provide significant advances in the long run. The study of the statistical correlations, the phase transitions, the associated type of ordering, etc, will provide another example of deepening our basic knowledge in the field. In particular, the role played by the quantum fluctuations near a critical point, and in the context of a lower dimensionality, is a topical subject, of a steadily growing interest. Disordered magnetic systems, quantum fluids, critical fluctuations near phase transitions will continue to be covered in the future. The experience acquired so far in the description of these systems enables also the enlargement of the applications to new fields such as biological, economical and social sciences. There is already an interesting progress in modelling important phenomena in such domains to justify the hope of performing specific investigations and predictions based on these models. New electronic phase transitions, as the two-band ferroelectric one, and their novel features, are expected to enlarge our knowledge of these basic phenomena. Linear response theories and the transport theories for quantum gases and liquids, multi-chain Luttinger liquid, phase hamiltonians, quasi-one-dimensional electronic solid and the quasi-classical methods of treating the condensed matter phenomena are also envisaged as long-term goals. Powerful and more flexible mathematical methods will also follow from these investigations, with relevance in various other fields of research, thus emphasizing the unitary character of the theoretical physics; it is worth remarking here the non-linear transport or master equations for complex systems, the travelling waves in constrained geometries, the overall behaviour of multi-degrees-of-freedom dynamics, etc. Atomic correlated multi-particle wavefunctions are also another long-term goal, as a prerequisite in condensed matter studies. The interpaly between stuctural transitions and spin dynamics, with reference to peculiar magnetic properties of certain compounds are also expected to provide a significant advance in the future; and, last but not the least, it is worthwhile mentioning here the development of powerful and refined methods of numerical analysis for the associated, complex mathematical problems.