Abstract

The applicant: B. Szafran from Krakow (Poland) intends to spend a year in the group of prof. François Peeters in Antwerp (Belgium). During the stay in Antwerp the applicant will consider theoretically the Wigner phase in the localization of quantum electron systems confined in semiconductor quantum dots. In the Wigner phase the electrons occupy separated space sites, which results in semi-classical properties of the quantum systems. The Antwerp group possesses the expertise in the study of the classical counterparts of the quantum systems to be considered in the present project. The applicant developed a method of solution of the Schroedinger equation which yields exact results in the high-magnetic field limit, in which the quantum system reproduces the classical type of localization. The applicant will benefit from the complementary expertise of the Antwerp group in the study of the Wigner localization. He will learn the Monte-Carlo techniques which were developed to study the phases of classical charged systems confined in semiconductor nanostructures. The method developed by the applicant uses a multicenter basis of the wave functions corresponding to the lowest Landau level. The centers of the one-electron wave functions will be optimized with respect to the total energy of the quantum system using the methods developed in Antwerp for the classical systems. The direct objectives of the project includes: determination of the mechanism of the maximum density droplet breakdown and of the formation of the Wigner phase in quantum dots, quantum rings and wires, discussion of the Wigner phase in systems with broken symmetry and in large quantum dots with disorder induced by the local fluctuation of the confinement potential. The applicant will study the liquid-solid as well as solid-solid phase transitions induced by external fields in the quantum systems considered. In Antwerp the applicant will obtain training in the determination and qualification of the phase transitions. The theoretical results obtained during the realization of the project will be compared with the experimental data of the transport and capacitance spectroscopy [Oosterkamp *et al*., Phys. Rev. Lett **82**, 2931 (1999), Zhitenev *et al.*., Phys. Rev. Lett. **79**, 2308 (1997)]. In particular the applicant intends to explain the additional cusps of the charging spectra of vertical quantum dot of Oosterkamp *et al.* which appear in magnetic fields above the maximum density droplet stability regime. Moreover, the applicant will estimate the influence of the disorder on the formation of the Wigner phase and simulate the changes in the electron distribution induced by the external magnetic field. This study will verify the hypothesis of the existence of local puddles of electron localization induced by the disorder and estimate the role of the screening of the electron-electron interaction by the external electrodes in bunching of the charging spectra as function of the external magnetic field [c.f. Zhitenev et al]. The project will be realized using the unrestricted Hartree-Fock method and a novel configuration interaction scheme which will be based on the exact solutions of the few-electron Schroedinger equation in the high-magnetic field limit. The applicant will learn the current spin density functional theory, which is used in the Antwerp group. The expertise gained in this training will allow the applicant to generalize his past experience in simulation of the vertical quantum dot of Tarucha *et al.* [Tarucha *et al.* Phys. Rev. Lett. **72**, 3613 (1996)] to novel nanodevices with arbitrary geometries. The project will be realized in cooperation with prof. F. Peeters as well as with several post-docs and PhD students working in Antwerp. The realization of the project-specific objectives will enable the applicant to prepare a dissertation (equivalent to German habilitation) which will allow him to gain formal scientific independence at his home university in Krakow, where he is employed as the permanent researcher. The auxiliary training, especially in the current spin density functional theory will be crucial for the future independent career of the researcher. The applicant in future should serve as a link in the cooperation of the Krakow group with the group of Antwerp.

B1. Scientific quality of the project

B1.1 Research Topic: Wigner Phases in Quantum Dots

A theoretical study of the Wigner phase of electrons confined in semiconductor quantum dots will be performed. Semiconductor quantum dots are nanostructures in which charge carriers are confined in all three directions resulting in a discrete atomic-like energy spectrum [1-3]. For this reason these systems are called *artificial atoms* [4]. They have been extensively studied theoretically and experimentally over the last decade because of their novel physical properties as well as because of their possible application in nanoelectronics, optoelectronics and quantum computing. In particular, the quantum dots have been used as a prototype of a single-electron transistor [5], they have been proven to be useful in construction of light-emitting and laser diodes [6] and they are considered as one of the possible realizations of a qubit in a potential implementation of a solid-state quantum computer [7].

The Wigner phase is a strongly correlated state of electron system in which the electrons occupy distinctly separated sites in space. As a consequence of the separation of the electron charges in the Wigner

phase, the quantum electron system exhibits a semi-classical type of localization. Wigner predicted [8] in 1934 a phase transition between the electron-liquid and the electron-solid phase (Wigner crystal) for a three-dimensional low-density electron system. Such a Wigner crystal was observed [9] by Grimes and Adams in 1979 in a two-dimensional system of electrons confined on the surface of liquid helium. This is the Wigner crystal in the low-density classical regime. Formation of a two-dimensional quantum Wigner crystal was reported [10] 10 years later on a GaAs/GaAlAs heterojunction in the quantum Hall regime. The latter is realized in strong external magnetic fields for which the Landau-level filling factor is lower than about 0.2 [10]. A pinned Wigner solid was subsequently observed [11] in a Si MOSFET in the absence of a magnetic field.

The Wigner phase in quantum dots is called a Wigner molecule or a Wigner cluster. It has been predicted to appear spontaneously in large structures, at low electron density [12-15]. It has also been shown theoretically that the Wigner molecules can be induced by a strong external magnetic field in nanostructures [16-23]. The external magnetic field leads to spin polarization of the electron system confined in the quantum dot. The state, which appears just after the appearance of the spin polarization, called a maximum density droplet (MDD) [24], is characterized by an electron density distribution with a single flat extremum. In this extremum the electron density is uniform. An increase of the magnetic field leads to a breakdown of the MDD [25,26]. The breakdown of the droplet has been observed [27] in vertical quantum dots. After the breakdown of the MDD, the Wigner molecule phase is formed [16,19,23]. So far, different theoretical approaches have been proposed to describe the Wigner molecule phase in quantum dots: unrestricted Hartree-Fock [15,16,18,23], exact diagonalization schemes [20,24] and current spin density approach [19]. At present all the authors seem to agree, that in the high-field limit the shape of the Wigner molecule phase can be derived from the classical considerations [28,29]. However, different scenarios of the MDD breakdown have been reported. Reimann *et al.* [19] claim that the breakdown appears from the edge of the MDD, where a ring of separately localized electrons emerges from a flat density maximum. This is in contrast with the theoretical results of Yang and MacDonald [22] who found that a hole is formed in the center of the dot, which breaks up the droplet. Szafran *et al.* [23] pointed out the possibility of the formation of the Wigner molecule just after the breakdown of the MDD and that this Wigner molecule has a different shape than in the high field limit. According to the latter results [23], the electrons prefer to stay at the outer surface of the Wigner molecule rather than in its center, which is then consistent with the conclusion of Yang and MacDonald [22]. However, the exact mechanism of the breakdown of the MDD remains an open question.

B1.2 Project objectives

The aim of the proposed project is to investigate Wigner molecules in quantum dots and related confined systems like ring and wire structures.

The main objective of the project is **the determination of the exact scenario for the breakdown of the maximum density droplet**, which is at present one of the most interesting problems in the field (c.f. B.1.1). There exist a controversy about the mechanism at which the MDD is transformed into a Wigner molecule at high magnetic field. A mechanism of edge reconstruction has been proposed [19] within the frame of the local current spin density approach. In this mechanism, first the charge density of electrons at the outer ring of the MDD crystallizes, leaving the inner surface of the droplet unchanged. The opposite mechanism was predicted by the unrestricted Hartree-Fock approach [23] and by the exact diagonalization [24] scheme, which indicate that there is an intermediate stage of crystallization, which appear between the MDD and the high-field semi-classical limit where a hole in the center of the charge density appears. According to our present knowledge these two scenarios [19, 23-24] are not necessarily contradictory. Instead, the first one [19] seems to be more suitable for a large number of electrons, i.e. N> 15, the other one [23,24] may be realized for smaller number of electrons. The objective of the project is to verify this hypothesis. This objective will be realized at two different stages. The first stage of the project will consist of the development of the already existing unrestricted Hartree-Fock theory and apply it to dots containing a small number of electrons. Subsequently, we will rely on the configuration interaction method, which allows for the exact solution of the few-electron Schroedinger equation.

The second objective of the project is **the study of the Wigner phase in structures with anharmonic and anisotropic confinement.** Most of the present studies have been performed for electron systems confined with two-dimensional cylindrical symmetric harmonic-oscillator confinement potential [18-24]. The electron systems in this potential can be relatively easy investigated because analytical exact solutions of the single electron problem in an external magnetic field are known (Fock-Darwin states). The exact solutions of the Schroedinger equation for cylindrically symmetric confinement may possess a rotationally invariant charge density [19,30]. The broken-symmetry solutions obtained within the mean field methods map the exact solution on a space restricted by the Hartree-Fock or local density approaches [19,30]. On the other hand a small anisotropy of the confinement potential should stabilize the exact charge density under a fixed angle in the

laboratory frame of reference [19]. The rotationally invariant solutions of the Schroedinger equation can be reconstructed from the broken Hartree-Fock results [30]. The importance of the charge density symmetry of Wigner phases in this frame of reference will have to be explained in this point of the project. We will determine the correction to the ground state energy, which is obtained when the rotational symmetry of the ground state is restored as function of the strength of the electron-electron interaction. The study of Wigner molecules in systems with anisotropic or anharmonic confinement would be a step towards more realistic structures. This study requires a method, which requires neither harmonicity nor cylindrical symmetry of the confinement potential. We have developed such a method [23], which can be readily applied to these problems. Phase diagrams for the ground-state configuration of the Wigner molecule as functions of the magnetic field, anharmonicity and anisotropy will be determined. As a straightforward generalization, we plan to investigate the Wigner phase in quantum rings and quantum wires. The Antwerp group determined [29] a number of such phase diagrams for classical systems confined in quantum dot, quantum wire and quantum rings as functions of the geometry of the confinement, form of the electron-electron interaction and the electron charge density. In the present project a study of the quantum phase diagrams is proposed.

A third objective of the project is the **estimation of the influence of disorder in Wigner molecule formation in quantum dots**. The presence of the random perturbation of the confinement potential should enhance the formation of the Wigner phase in quantum dots. Such perturbation, due to imperfections of the structure and the presence of the impurities in the neighborhood of the dot is present in vertical quantum dots produced by the group of Ashoori [32]. These dots are particularly large and the gate-induced confinement potential is relatively weak, which creates a possibility [32] that the electrons become localized in different local minima of the potential. We plan to study the magnetic-field induced localization of electrons in these random minima. The spread of the electron wave function in the lowest Landau level is decreased by the external magnetic field. Thus one should expect that at higher magnetic fields the electrons will be able to fit in the local fluctuations of the potential, while in the lower magnetic fields the electron wave function should be spread over the entire quantum dot. The magnetic field induced localization of electrons in the random fluctuations of the potential results in bunching of the charging lines observed in capacitance spectroscopy [32]. This bunching indicates that at high magnetic fields several electrons can enter the dot at once. This may happen if each of the electrons is localized in different ‘puddle’ and if the interaction between the ‘puddles’ is screened by the presence of a nearby electrode. We plan to verify this mechanism theoretically, as well as to determine the influence of the random fluctuations of the potential on the Wigner molecule formation.

B1.3 Scientific originality and innovation

The scientific originality and innovation of the proposed project consist in the development of a very promising method of treatment of the Wigner phase in quantum dots. We intend to use this method in order to explain unclear points in the theory as well as to study systems, which are hardly treatable with the existing state-of-art methods.

Extensive theoretical studies of Wigner molecules in quantum dots were motivated by the observation of the breakdown of the MDD in vertical gated quantum dot reported by Oosterkamp *et al.* [27]. The authors of the experiment [27] have identified the cusps in the charging spectrum, which correspond to the formation and the breakdown of the MDD. The experimental data [27] indicate that the breakdown appears abruptly which indicates that at a certain magnetic field the MDD is instantaneously transformed into the Wigner molecule. This experimental fact denies the smooth continuous edge-reconstruction mechanism of the breakdown [19]. Besides the cusp of the charging line attributed to the MDD breakdown, the experimental spectra contain additional structure appearing at magnetic fields after the MDD breakdown. This structure may be due to intermediate Wigner molecules, which can possess different symmetries in different magnetic fields [23]. The additional structure of the cusps contain both the cusps which change regularly with the number of electrons as well as a isolated cusps, which appear for N electrons and are absent for N-1 and N+1 particles. The latter cusps may be due to the transformations of the Wigner molecules, since the magnetic fields inducing these transformations do not seem [23] to exhibit regular dependence on N. The exact mechanism of the MDD breakdown and the additional structures of cusps appearing beyond the MDD stability regime until now are not completely understood (see. B1.1 and B 1.2). The first objective of the project is aimed to explain these effects, which would make a serious advance of the state-of-the-art knowledge of this field.

The starting point for the studies proposed in the present project is a novel multicenter basis for the Wigner molecule phase, which has been used in three very recent papers [21,23,30]. In the majority of the papers based on unrestricted Hartree-Fock and all the existing configuration interaction approaches, the magnetic field induced Wigner molecules are treated starting from the low-magnetic field limit [16,18,20,22]. Namely, the authors [16,18,20,22] use as a basis the eigenfunctions of the problem of a single electron confined in a harmonic

oscillator potential in the presence of an external magnetic field (Darwin-Fock states). This basis is suitable for the description of few-electron states at low magnetic fields but its fundamental shortcoming is its slow convergence in the high field regime [19], for which the exact electron wave functions exhibit a point-like localization. On the other hand, the multicenter basis [21,23,30] uses the exact lowest-Landau-level eigenfunctions, which can be centered on an arbitrary point in space. This basis allows for the exact description of the high-field classical limit of the Wigner localization. Moreover, we have shown [23] that the unrestricted Hartree-Fock with the multicenter basis allows for the description of the cylindrically symmetric MDD phase. A novel method, which will be elaborated during the project, is the configuration interaction approach within the multicenter single-electron basis. In this approach the basis for the many-electron calculations will be constructed from Slater determinants corresponding to electrons occupying different separated space sites. This new method should lead to a definitive resolution of the problem of intermediate phases appearing at the MDD. It will also provide an opportunity to study the border between classical and quantum mechanics (for explanation see point B.1.4).

The Hartree-Fock approach and the multicenter configuration interaction method, which will be elaborated during the execution of the first objective, will be used for the description of the magnetic-field induced Wigner molecules in structures with broken cylindrical symmetry and in cylindrically symmetric structures with anharmonic confinement potential. These models represent an important step from the idealized harmonic oscillator confinement towards realistic structures. The problem of the magnetic field in the few-electron systems confined in potentials with broken cylindrical symmetry is difficult by itself. The extreme, Wigner phase solutions are even more challenging. So far only low-electron density Wigner molecules in the absence of an external magnetic field have been studied in broken symmetry structures. However, the novel methods described briefly here and more extensively in point B1.4, are suitable for the study of these systems. In particular, the notion of the MDD will be generalized to systems with an anharmonic confinement potential and broken symmetry. We plan a description of the magnetic-field induced formation of a Wigner solid in quantum wires and quantum rings.

The disorder should enhance the formation of the Wigner phase in quantum dots. This interesting problem has not been studied so far and is planned as the third objective of the project. This study should allow for description of the localization/delocalization transition induced by the external magnetic field as well as for a qualitative interpretation of the experimental results [32] for the bunching of the charging lines. The importance of the screening of the interaction of electrons localized in different potential minima by the external electrodes will be estimated.

B1.4 Research method

The proposed project is based upon: 1) unrestricted Hartree-Fock (HF), and 2) the configuration interaction method. These methods allow for a straightforward solution of the few-electron Schroedinger equation. In the HF and the configuration interaction methods, the proper choice of a basis set of function is of crucial importance. The novel point of the calculations proposed in the present project is the use of the multi-center basis [21,23,30], which yields exact results in the high-field limit, i.e. in the regime where the Wigner phase exists in its extreme form of a semi-classical system of point charges.

In the high-magnetic field regime the confinement potential of a quantum dot can be neglected in a first approximation. The Hamiltonian for a single electron moving in an external magnetic field constructed with the Landau gauge **A**=(-*By*,0,0) has the form

$$h = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+2i\alpha y\frac{\partial}{\partial x}-\alpha^2 y^2\right), \qquad (1)$$

where m is the electron effective mass, $\alpha = eB/\hbar = m\omega_c/\hbar$, where ω_c is the cyclotron frequency. The lowest Landau level is infinitely-fold degenerate and its energy equals $E_0 = \hbar\omega_c/2$. Due to the infinite degeneracy of the lowest Landau level, the corresponding wave functions can be taken in many different forms. We choose the following one

$$\Psi_{\mathbf{R}}(x,y) = (\alpha/2\pi)^{1/2}\exp\left[-\alpha/4\left((x-X)^2+(y-Y)^2\right)-i\alpha/2\left(x-X\right)\left(y+Y\right)\right]. \qquad (2)$$

The charge distribution corresponding to (2) is a Gaussian centered at point **R**=(*X*,*Y*), which can be taken arbitrary, but which finally will be determined by the minimization of the total energy of interacting few-electron system. It is worth noting, that this charge distribution tends towards a point charge in an infinite large magnetic field. Functions of the form (2) can be used as a multi-center basis set for the solution of the unrestricted HF equations, as well as for the construction of the basis for the configuration interaction method. In our recent

paper we solved the Schroedinger equation for the *N*-electron system confined in a cylindrically symmetric harmonic potential, using this HF method, with the one-electron wave functions expanded in the multi-center basis

$$\Phi(x,y)=\sum_{i=1}^{N} c_i \Psi_{\mathbf{R}_i}(x,y) \ , \qquad (3)$$

where centers $\mathbf{R}_i$ were taken from the equilibrium position of classical charges, and the value of α in (2) was replaced by a variational parameter. We have shown [23], that the multicenter basis (3) is more suitable for the description of Wigner molecules in quantum dots than the commonly used [16,18,20,22] Fock-Darwin basis of functions centered at the origin, especially at high magnetic fields and for larger number of electrons. We have shown [23] that the basis (3) not only allows for the description of point-like localization at high magnetic field, but also mimics the cylindrically symmetric maximum density droplet (MDD) charge distribution with a surprising accuracy. Using basis (3) we have predicted [23] several shape transformations of the Wigner molecules. These transformations are due to the fact that the ground-state phase of the molecule as it emerges from the MDD phase may be different than in the classical high magnetic field limit.

A multi-center basis has been applied to Wigner crystals [31] in the unconfined two-dimensional systems. Recently Kainz *et al.* [21] have used a similar approach to the problem of Wigner molecules in quantum dots. Namely, they constructed a Slater determinant from wave functions centered at different centers. Their approach [21] is not equivalent to HF, since the occupied orbitals are not orthogonal in the case of an arbitrary magnetic field. In particular the two approaches produce different charge density. The method of Kainz *et al.* [21] does not allow for the description of the MDD and therefore it cannot account for the effects appearing at the MDD breakdown. However, this method [21] becomes equivalent to the HF method when a sufficient large magnetic field induces a spatial separation of the one-electron wave functions, which then become orthogonal because of the lack of overlap. Yannouleas and Landman [30] showed that a construction of the states with rotationally invariant charge density could be obtained from the mean-field broken symmetry solutions obtained in a basis of type (3).

The HF method works with a different precision for states with different spin-orbital configurations. In particular, it works with a much higher precision for spin-polarized states then for unpolarized states. The electrons in the Wigner molecule in the presence of a high external magnetic field as well as in the MDD phase are spin-polarized. Therefore, one should expect that the HF method works with a relatively high precision for both the Wigner and the MDD phase. Mueller and Koonin [16] have shown that in the limit of high magnetic field the unrestricted HF results for the energy estimation cannot be significantly improved. The accuracy of the HF method for the MDD was pointed out by MacDonald *et al.* [1993]. Therefore, in the high magnetic field the unrestricted Hartree-Fock with properly chosen basis provides an exact solution of the Schroedinger equation. However, at finite magnetic fields, in the MDD regime and in the range of magnetic-fields for which shape transformations of the Wigner molecule are predicted [23], an improvement of the results is still possible both within the frame of HF as well as by the configuration interaction method.

The improvement of the variational estimates of the ground-state energies within the HF method can be realized by a generalization of the basis (3). This generalization can and will be performed as follows:

1) A separate variational parameter α can be introduced for the real and imaginary term in the exponent of formula (2). Moreover the parameters can be made position dependent. Such wave functions could simulate the edge reconstruction scenario for MDD breakdown [19]. The positions of the centers of the basis (3) were previously taken [23] from scaled classical configurations. Now we will optimize their positions with respect to the total energy of the quantum system. In this point we will use the Monte-Carlo methods developed in Antwerp [29] for the treatment of the classical Wigner molecules.
2) Basis (3) uses one function (2) for each of the electrons. Using more than one function per electron should improve the results.
3) Basis (3) contains only wave functions corresponding to the lowest Landau level. Functions corresponding to the first excited Landau level will be added.
4) Reconstruction of the rotationally invariant charge density based on the solution of the HF equation will be performed in order to estimate the importance of the symmetry of the charge distribution in the laboratory frame [19,30] (see. point B.1.2).

A step beyond HF should allow for a more precise estimation of the total energy in a finite magnetic field. At finite magnetic field, the HF results can be improved by the configuration interaction approach. In the HF method the few-electron wave function is expressed as a single Slater determinant built from orthogonal wave functions. In the configuration interaction approach many Slater determinants corresponding to different configurations are used as a basis. In the present project we plan to develop a configuration interaction method

with basis corresponding to various shapes of the Wigner molecules. We expect that in the high field limit the variational method will choose one, namely, the lowest, classical configuration of charges. At lower magnetic fields this method should account for mixing of Wigner molecules of different shapes. We have shown [23] that the ground state configuration of the Wigner phase may change several times as the MDD breaks down. In the magnetic field just above the breakdown the different spatial configurations of the Wigner molecules correspond to very similar energies. Moreover the wave functions of different configurations at finite magnetic fields are not orthogonal. Therefore, we expect that at the droplet breakdown, many configurations may contribute to the description of the exact few-electron wave function. The configuration interaction method based on the distribution of electrons among different space sites would be the first of its kind. It would offer a possibility of a definitive solution of the problem of intermediate Wigner phases appearing at the breakdown. In classical mechanics only a single configuration with a well-defined shape is realized, while quantum mechanically a superposition of different shapes can be realized. The configuration interaction method which will be developed in the proposed project offers also an opportunity to study the transition between the classical and quantum Wigner configurations.

The results obtained with the HF and exact diagonalization methods developed during the execution of the present project will be compared with the results of the density functional theory (DFT). This comparison is necessary, since both the approaches predict different mechanisms of the MDD breakdown. We plan to use the numerical DFT programs, which were developed in Antwerp [33] in collaboration of the applicant with B. Partoens and F. Peeters. The Antwerp group possess expertise [33] in the current spin density functional theory which is suitable for the treatment of the electron systems in external magnetic field, as well as in the application of the local density approximation in the study of the phase of the Wigner crystals in electron bilayers.

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B2. Quality of the research training

The applicant will be trained in two principal points: Monte-Carlo (MC) methods for the description of the classical Wigner molecules and the density functional theory (DFT). The successful realization of the objectives of the proposed project requires expertise in these fields. The Antwerp group possesses this expertise. The applicant needs training in MC and DFT since these methods were never applied by his home Krakow group.

The proposed theoretical approach to treat the confined electron systems with the multicenter basis set requires a proper choice of the centers of the one-electron wave functions (c.f. B 1). The Antwerp group worked on the classical counterparts of the quantum systems, which are to be studied in the proposed project. In particular, the Antwerp group possess a long-term experience and expertise in the methods of finding the stable, metastable and saddle-points of the classical Wigner crystals and molecules in structures with different dimensionality and shape. The MC methods developed in Antwerp can be directly applied to the quantum problems, if the total energy of the quantum system replaces the potential energy of the classical system. The objectives of the present project include the study of the liquid-solid phase transition which appears when the maximum density droplet breaks down and transforms into the Wigner molecule, as well as the study of the solid-solid transitions which appear when the ground-state of the electron system in a Wigner phase changes its spatial shape. The project includes the discussion of the quantum phase diagrams for the Wigner molecules in function of the external fields, geometry of the quantum dots, and type of the confinement potential including random fluctuations introduced by the disorder. In Antwerp, the applicant should learn how to generate numerically the studied phases. The applicant should also profit from the expertise of the Antwerp group in the determination and qualification of the phase transitions.

The applicant possesses the expertise in the exact diagonalization and Hartree-Fock (HF) methods for the solution of the Schroedinger equation for the few-electron systems, but he has never applied DFT, which is one of the approaches used in Antwerp. One of the objectives of the proposed project is the explanation of the different phase diagrams obtained with the current spin density functional theory (CSDFT) and the HF - exact diagonalization approaches. This explanation will require the application of the CSDFT to the problem of the decay of the maximum density droplet. The Antwerp group has used this particular DFT method to the problem of electron systems in external magnetic field, so the applicant should obtain a suitable training in this approach. He will also be able to use the programs developed in Antwerp in collaboration with B. Partoens and F. Peeters. The Antwerp group has used the DFT for the description of the phase transitions in quantum electron systems in bilayers, including the liquid-solid transition and transition between different phases of Wigner crystals in these systems. The applicant has an experience in the study of the Wigner molecules confined in quantum dots, but he has never studied systems with higher dimensionality. He will obtain training in the treatment of the infinite systems, including bilayers and quantum wires.

The applicant has an experience in simulating the nanodevices. In particular, he has worked on the solution of the Poisson-Schroedinger problem for the vertical quantum dot of Tarucha et al. (c.f. B 4). The Schroedinger equation for the quantum-dot-confined electron system was solved with the HF method. The generalization of the Poisson-Schroedinger scheme on more complex systems, i.e. systems of multiple quantum dots and systems with lower symmetry, requires the application of the DFT instead of HF, which is not suitable for a time-effective flexible differential schemes, because of the form of the exact exchange interaction. The expertise in DFT, which the applicant hopes to acquire in Antwerp, will enable him to perform simulations of arbitrary devices of the nanoelectronics, which would be crucial for the future independent career of the applicant.

The applicant works as a teacher of the computational physics at his home University in Poland. Therefore, besides the scientific interest, the expertise in MC and DFT will be useful for the applicant as a teacher. The auxiliary training that the applicant will find in Antwerp is the capability of working in a large international team. The applicant will learn Flemish language.

B3. Quality of the host

B3.1 Scientific and training expertise of the host

The center of gravity of the research at the Physics Department of the University of Antwerp (UA) is in material science and condensed matter physics. The department also organizes a ‘master in nanophysics’.
There are six different research groups at UA in this area: 1) Electronmicroscopy for material research, 2) Theoretical study of matter, 3) Experimental physics of condensed matter, 4) Theoretical solid state physics, 5) Condensed matter theory, and 6) Theory of molecular materials.

The Antwerp theory group: *Condensed Matter Theory* (CMT) will be the host for Dr. B. Szafran, and is directed by: Prof. dr. François Peeters.
Currently, the group consists of: 1 visiting professor, 9 postdocs and 9 PhD-students.
On its www-site (http://hipe.uia.ac.be/cmt) information is available about: the members of the group, research subjects, computer infrastructure, list of publications, and the courses, seminars and workshops which are organized.

The host research group is funded by projects from: i) Antwerp University ('Gemeenschappelijke Onderzoeksraad Antwerpen' and the 'Bijzonder Onderzoeksfonds'), ii) Belgium (the Flemish Science Foundation; the Institute for Science and Technology; Belgian office for scientific, technical and cultural affairs; Bilateral Scientific and Technological collaboration), and iii) Europe (INTAS, ESF-network, EU-growth program and Marie Curie program (RTN-network and individual fellowships).

The group **publishes** yearly typically about 20 papers in international journals (e.g. PRL, PRB, PRE, Nature, APL, JAP, J. of Physics: Cond. Matter, SSC) and about 18 papers in conference proceedings.

The host institute collaborates and has **collaborated internationally** with several groups. Only those collaborations are mentioned which have resulted in joint publications.
Collaboration with experimental groups: VSM/KULeuven, IMEC (Leuven), TUE (Eindhoven), Nijmegen (The Netherlands), Clarendon (Oxford), Nottingham (UK), Manchester (UK), Linz (Austria), Grenoble (France), Buffalo (NY, USA), Tallahasee (USA), Tokyo (Japan), Chernogolovka (Russia).
Collaboration with theoretical groups: Athens (Ohio, USA), Davis (California, USA), Montréal (Canada), Ottawa (Canada), Hokkaido (Japan), Berlin (Germany), Krakow (Poland), Alicante (Spain), Prague (Czech Republic), Novosibirsk (Russia), Debrecen (Hungary), Szeged (Hungary), Vilnius (Lithuania), Belgrade (Yugoslavia), Yerevan (Armenia), Wollongong (Australia), São Carlos (Brazil), Fortaleza (Brazil), Beijing (China), Habana (Cuba), Tel Aviv (Israel), Beer-Sheva (Israel).

There exist regular contacts with the candidate’s group which is headed by Prof. J. Adamowski. This has led to regular visits by him to Antwerp resulting in joint publications.

Participation in projects:
The host participated in the past to: COST-actions (‘Mesoscopic electronics’), Phantoms (EU-network in IST), INTAS, HCM-network, NATO grants)
Research projects currently funded by Belgium funding agencies:
- “Correlations in Coulomb interacting systems” (Flanders-Hungary collaboration); 2001-2004
- “Spintronics” (Flanders-China collaboration); 2001-2004
- “Structure and dynamics of vortices and charged particles in mesoscopic confined systems”; 2002-2005
- “Magneto-optical studies of exciton complexes and quantum mechanical coupling for improved quantum dot laser design”; 2001-2003
- “Mesoscopic and nanophysics of semiconductors and superconductors”; 2000-2003
- “Confinement phenomena in nanostructured superconductors”; 2000-2003
- “Spin correlations and spin dependent transport in high magnetic fields”; 1999-2003
- “Nanostructures: electronic, magnetic and optical phenomena”; 1999-2004

Currently funded European projects:
- CERION-2 (Canadian European Research Initiative on Nanostructures - 2); 2002-2004
- “Theoretical research on charge correlation in low dimensional systems” (Marie Curie Training side); 2001-2004
- “NANOMAT: Self-assembled nanostructured Materials for electronic and optoelectronic applications” (EU-growth program); 2001-2004
- EU-RTN on: “Surface electrons on mesoscopic structures”; 2000-2004

- "Vortex matter in superconductors at extreme scales and conditions" (ESF-network); 1998-2003

The above European 'RTN' and 'training site' projects, which are coordinated by the host, have **training** as an essential component. Previous postdoctoral fellowships awarded to the host by the EU:

- Marie Curie fellowship: Dr. E. Anisimovas: "Many-body effects in the dynamical properties of bilayer electron systems" (2001)
- Human Capital and Mobility (individual fellowship): Dr. V. Karavolas: "Multi-subband electronic transport in systems of reduced dimensions" (1993)

Currently, 3 post-docs and 4 PhD-students, supervised by F. Peeters, are working in the area relevant to the project of Dr. Szafran.
Total number of PhD-students supervised by F. Peeters: 14

Expertise in the area of quantum dots:
The first paper by the host on quantum dots was published as a rapid communication in PRB where he proved Kohn's theorem for parabolic confined elliptical quantum dots (F.M. Peeters, Phys. Rev. B **42**, 1486 (1990) – this paper has already 90 citations). After this initial paper the subject of quantum (and classical) dots was a major field of research for F. Peeters. In 2002 his group published 10 papers in this area.
Recent key papers from the host relevant to the project of Dr. Szafran:

- B. Partoens and F.M. Peeters: *Magnetic field induced spin and isospin blockade in two vertically coupled quantum dots*, Europhys. Lett. **56**, 86-91 (2001).
- B. Partoens and F.M. Peeters: *Molecule-type phases and Hund's rule in vertically coupled quantum dots*, Phys. Rev. Lett. **84**, 4433-4436 (2000).
- K.L. Janssens, B. Partoens, and F.M. Peeters: *Stark shift in single and vertically coupled type I and type II quantum dots*, Phys. Rev. B **65**, 233301 (2002).

The expertise of CMT relevant for the project of Dr. Szafran is on: 1) density functional theory, 2) exact diagonalization of finite particle systems, 3) Monte Carlo simulation of classical systems, and 4) finite difference techniques.

The applicant will obtain **training** in the following areas:

- *Project specific.* The applicant will be trained in new *numerical techniques*: like finite-difference techniques, numerical simulations (Monte Carlo and molecular dynamics), and density functional theory. The latter can be provided within the CMT group but also through the bilateral (Flanders-Hungary) project which includes other theory groups (physics and chemistry) in Belgium and the the Psi-k ESF-network to which CMT participates. Regularly, CMT organizes a 10 lecture course (with practical sessions) on programming in 'C++ and Object Oriented Programming'. This course is open to all the PhD-students and postdocs of the university. There is also the possibility to follow topical courses at CECAM (Lyon) where CMT has close links to.
- *Non-project specific and interdisciplinary*. CMT organizes regular seminars and minicourses: e.g. a `minicourse on biophysics' was organized in January 2001. Each year an interdisciplinary (in collaboration with the chemistry department) one week course is organized on different topics of `materials science'. On a weekly basis there are group seminars where the applicant is expected to participate actively through e.g. his own contributions.

The applicant is expected to collaborate with post-docs and PhD-students of the CMT group, in particular M. Tavernier, M. Kong, Dr. B. Partoens and Dr. E. Anisimovas.
He is expected to contribute to the existing NANOMAT-project and to one or more of the bilateral exchange projects (with China and Hungary) in which the group is involved.

B3.2 Quality of infrastructure

Scientific:

- Library: the most important journals in physics are available or can be consulted through the internet. E.g. full access to all journals by Elsevier, the most important APS journals like e.g. all Physical Review journals, Applied Physics Letters, Journal of Applied Physics, Europhysics Letters, …
- Computer infrastructure An extended computer infrastructure is available consisting of: a 8 node dual processor (intel Xeon 2.4 GHz) PC-cluster, 4 workstations/servers and 22 stand alone PC's (at least Pentium-III) for individual use and connection to the local network and to internet.

Local arrangements:

- The group of the host provides each PhD-student and postdoc with the necessary office space which includes a private desk and a PC (at least Pentium III) with connection to the local network, internet and electronic library access.
- The university of Antwerp has a social service which not only takes care of problems related to visa, passport and lodging but organizes also regular activities (cultural, sports, visits) for foreign visitors and students.

This infrastructure should be sufficient for a theoretical researcher to complete his project.

B4. Quality of the researcher

The topic of the research project deals with a theoretical description of the Wigner localization of electron systems confined in quantum dots. Dr. Bartlomiej Szafran has been working in the field of research for several years. His master diploma and his thesis were devoted to the study of electron systems in quantum dots. Dr. Szafran gained an expert knowledge of the field and serve as a referee for several journals. The technical points of the project require solution of the Hartree-Fock equations and construction of the configuration interaction method. Dr. Szafran is certainly able to manage these problems. He is a coauthor of several papers [7a-9a,11a-14a,16a-17a,21a-23a,28a-29a] using the Hartree-Fock approach. Recently he has developed the configuration interaction method dedicated to three-dimensional electron systems confined in vertical quantum dots [30a]. Moreover, he has already started working on the Wigner phase in quantum dots [29a].

Three major achievements of the applicant are: (I) the description of the charging spectra of three-dimensional cylindrical quantum dots [16a,17a], (II) determination of the energy spectrum and symmetries of excitons in coupled quantum dots [24a,25a], (III) participation in the creation of the theoretical model [7a,11a-14a,21a-23a,28a,30a] of the gated quantum dot [S. Tarucha *et al.* Phys. Rev. Lett. **77**, 3613 (1996), L.P. Kouwenhoven *et al.* **278**, 1788 (1997)].

(I) Most of the quantum dots possess a flat shape, i.e., the confinement in the vertical dimension is much stronger than the lateral one. Then, all the occupied single-electron energy levels correspond to the same state of quantization in the vertical direction. In this sense the vertical degree of freedom is frozen and all the interesting effects appear at the plane of vertical confinement. This fact is at the origin of the two-dimensional models of quantum dots. However, in strictly two-dimensional models the Coulomb interaction between the electrons is enhanced and overestimated. The purpose of this project [16a,17a] was the description of the single-electron charging spectrum for the artificial atoms with confinement potential modeled as a three-dimensional finite quantum well of cylindrical shape. The Hartree-Fock method was used in order to calculate the dependence of the chemical potentials on the external magnetic field. The limits of applicability of the two-dimensional approximation have been determined [16a,17a]. The critical height to radius ratio for which the second state of quantization of vertical motion intervenes in the few-electron spectrum has been found. The applied model allowed for quantitative description of the single-electron charging spectrum of self-assembled quantum dots measured with the capacitance spectroscopy [B.T. Miller *et al*. Phys. Rev. B **56**, 6764 (1997)]. Such a description was not possible in the two-dimensional model without breaking its consistency [R.J. Warburton *et al*. Phys. Rev. B **58**, 16221 (1998)].

(II) The aim of this work [24a,25a] was a determination of the neutral and charged exciton spectrum of vertically coupled quantum dots. A simple phenomenological model was developed for InGaAs self-assembled quantum dots embedded in the GaAs, based on an assumption of a Gaussian distribution of indium concentration in the dot. The Gaussian function of indium distribution was supposed to determine the space-dependence of the electron and hole effective masses as well as the valence and conduction band offsets and thus describe the confinement potential for electrons and holes. The parameters of the Gaussian distribution were extracted from the experimental photoluminescence data for isolated dots [S. Fafard *et al.* Appl. Phys. Lett. **76**, 2268 (2000)]. These data were then applied without a further adjustment to study the exciton spectrum in vertically stacked coupled quantum dots in function of the thickness of the interdot spacer. A good agreement with the experimental data has been obtained. The appearance of the additional spectral lines in the strong coupling limit has been predicted. The problem of the parity symmetry of the excitonic wave function has been discussed. It has been shown that the one-particle parities are approximately conserved only in the strong coupling limit.

(III) The largest project dr. Szafran have been involved in is the numerical simulation [7a,12a-14a, 21a,23a,28a,30a] of the vertical quantum dot of Tarucha *et al.* [Phys. Rev. Lett. **77**, 3613 (1996)]. The project has been performed for last five years as teamwork of S. Bednarek, B. Szafran and J. Adamowski. Dr. Szafran was responsible for the solution of the three-dimensional Schroedinger equation for the confined electron

system. This equation was solved with unrestricted Hartree-Fock method, which was recently partially replaced [30a] by the configuration interaction method. The measurements performed on the device of Tarucha *et al.* provided the finest picture of the Coulomb blockade, shell-filling effects, co-tunneling, Kondo effect, the magnetic-field-induced evolution of the confined electron system including the breakdown of the maximum density droplet and formation of a Wigner molecule. This device inspired a very large number of theoretical papers. The experimental data exhibited a strong nonlinear dependence of the voltage-to-energy conversion factor on the potential of the gate. This dependence inhibited a quantitative comparison of the experimental data with the results of theoretical calculations, which neglected the electrostatics of the entire device. In this project the problem of the electrostatics has been definitively solved [23a,28a,30a]. The theoretical description of the electrostatics was difficult because the lateral confinement potential of electrostatic origin was influenced by a number of factors: the geometry of the device, the doping profile, the effects on the metal/semiconductor interface, and the applied voltages. Moreover, the confined charge and the space charge of ionized impurities in n-GaAs layers where coupled by the Coulomb interaction. Therefore, the Schroedinger-Poisson problem had to be solved for the entire nanodevice. The calculations [23a,28a,30a] gave a fine description of the shell-filling effects and the stability diagram (Coulomb diamonds). The calculated magnetic-field dependence of the charging lines exhibited systematic deviations from the experimental data. As it has recently been shown [30a] these deviations were due to the tendency of the Hartree-Fock to favor spin-polarized states. The application of the exact diagonalization scheme [30a] gave an impressive agreement with the experimental data. The calculations provided a deep insight into the physics of the vertical quantum dot, the shape of the confinement potential, the gate-voltage-to energy conversion factor, the distribution of the charge in doped GaAs layers and on the electrodes, the electron-electron correlation effects and the screening of the electron-electron interaction by the charges external to the dot.

Dr. Szafran worked on several problems involving quantum dots: donor systems [1a-6a,19a], electron-phonon coupling [5a-6a], theory of artificial atoms [7a-10a], numerical simulation [7a,12a-14a,21a,23a,28a,30a] of the vertical quantum dot of Tarucha *et al*., neutral and charged excitons [15a,24a,25a,27a], coupled quantum dots [24a,25a], electron-electron correlation [20a,30a]. Dr. Szafran is the first author of the majority of his papers, which reflects his initiative and the leading role in these projects. At present dr. Szafran is a supervisor of five student master degree projects, which also reflects the leadership of the young researcher.

In his past experience dr. Szafran was connected with a group of prof. Bernard Stébé of University of Metz (France) and with a group of prof. Janusz Adamowski of AGH University of Mining and Metallurgy in Kraków (Poland). He has obtained the master and PhD degrees of both the universities. At present dr. Szafran gained position of permanent researcher at the AGH University in Kraków. Dr. Szafran is a high quality young researcher which was recognized by several prestigious awards. Namely, he obtained the most prestigious Polish award for the thesis – the Prime Minister Award, which is granted to about 30 PhDs each year, irrespective of the field of research. Moreover dr. Szafran obtained scholarship for the most promising young scientists of the Foundation for Polish Science (FNP) for 2001 and 2002. This scholarship is granted to about 15 physicists each year. The team composed of prof. Adamowski, prof Bednarek and dr. Szafran obtained twice (in 1999 and 2001) the Award of the Minister of the Education for the scientific achievements. Ten papers of dr. Szafran *et al.*, have been published in Physical Review B, which is one of the most prestigious journals in his field of research.

List of publications of the applicant

[1a] **B.Szafran**, J.Adamowski, B.Stebe *Ground and excited states of D- centres in semiconductor quantum dots* Mat. Sci. Forum **258-263** (1997) 1707
[2a] **B.Szafran**, J.Adamowski, S.Bednarek, B.Stebe *Influence of donor impurity on optical transitions in quantum dots* Phys. Stat. Sol. B**210** (1998) 677
[3a] **B.Szafran**, J.Adamowski, S.Bednarek, B.Stebe *Formation of bound electron pairs in semiconductor quantum dots* Molec. Phys. Rep. **21** (1998) 89
[4a] **B.Szafran**, J.Adamowski, B.Stebe *Energy spectrum of D- centres in spherical quantum dots* J. Phys.: Condens. Matter **10** (1998) 7575
[5a] S.Bednarek, **B.Szafran**, J.Adamowski, I.Essaoudi, B.Stebe *Phonon resonances in optical spectra of donors in quantum wells* Physica B**273-274** (1999) 947
[6a] **B.Szafran**, B.Stebe, J.Adamowski, S.Bednarek *Effect of the electron-phonon coupling on the ground state of a D- center in a spherical quantum dot* Phys. Rev. B **60** (1999) 15558
[7a] **B.Szafran**, S.Bednarek, J.Adamowski *Theoretical description of shell filling in cylindrical quantum dots* Acta Phys. Polon. A**94** (1998) 555
[8a] S.Bednarek, **B.Szafran**, J.Adamowski *Many-electron artificial atoms* Phys. Rev. B **59** (1999) 13036
[9a] J.Adamowski, **B.Szafran**, S.Bednarek, B.Stebe *Few-electron artificial atoms* Few-Body Systems Suppl. **10** (1999) 189
[10a] **B.Szafran**, J.Adamowski, S.Bednarek *Ground and excited states of few-electron systems in spherical quantum dots* Physica E**4** (1999) 1
[11a] **B.Szafran**, S.Bednarek, J.Adamowski *Theoretical analysis of magnetic-field-induced evolution of transport windows in a vertical quantum dot* Proc. 25th Int. Conf. Phys. Semicond, Osaka, 2000, p. 1085
[12a] S.Bednarek, **B.Szafran**, J.Adamowski, *MBE-grown gate-controlled quantum-dot nanostructure and its current-voltage characteristics* Thin Solid Films **367** (2000) 97
[13a] S.Bednarek, **B.Szafran**, J.Adamowski *Quantum Coulomb blockade in gate-controlled quantum dots* Microelec. Eng. **51-52** (2000) 99
[14a] S.Bednarek, **B.Szafran**, J.Adamowski *Solution of the Poisson-Schroedinger problem for a single-electron transistor* Phys. Rev. B **61** (2000) 4461
[15a] **B.Szafran**, B.Stebe, J.Adamowski, S.Bednarek *Recombination energy for excitonic trions in quantum dots* J. Phys.: Condens. Matter **12** (2000) 2453
[16a] **B.Szafran**, J.Adamowski, S.Bednarek *Single-electron charging of self assembled quantum dots* Thin Solid Films **367** (2000) 93
[17a] **B.Szafran**, J.Adamowski, S.Bednarek *Few-electron systems in quantum cylinders* Phys. Rev. B **61** (2000) 1971
[18a] J.Adamowski, M.Sobkowicz, **B.Szafran**, S.Bednarek, *Electron pair in a Gaussian confining potential* Phys. Rev. B **62** (2000) 4234
[19a] **B.Szafran**, J.Adamowski, S.Bednarek *Infrared optical versus transport spectroscopy for few-electron spherical quantum dots* J. Phys.: Condens. Matter **12** (2000) 6837
[20a] **B.Szafran**, J.Adamowski, S.Bednarek *Electron-electron correlation in quantum dots* Physica E**5** (2000) 185
[21a] S.Bednarek, **B.Szafran**, J.Adamowski *Induced-charge distribution in vertical quantum dots* Proceedings of SPIE **4413** (2001) 129
[22a] J.Adamowski, S.Bednarek, **B.Szafran** *Transport and capacitance spectroscopy of quantum dots* Acta Phys. Pol. A**100** (2001) 145
[23a] S.Bednarek, **B.Szafran**, J.Adamowski, *Theoretical description of electronic properties of vertical gated quantum dots* Phys. Rev. B **64** (2001) 195303
[24a] **B.Szafran**, S.Bednarek, J.Adamowski, *Parity symmetry and energy spectrum of excitons in coupled self-assembled quantum dots* Phys. Rev. B **64** (2001) 125301
[25a] **B.Szafran**, B. Stebe, J. Adamowski, S.Bednarek, *Excitonic trions in single and double quantum dots* Phys. Rev. B **66** (2002) 165331
[26a] M.Ciurla, J.Adamowski, **B.Szafran**, S.Bednarek *Modelling of confinement potentials in quantum dots* Physica E**15** (2002) 261-268
[27a] **B.Szafran**, J.Adamowski, S.Bednarek *Effect of the repulsive core on the exciton spectrum in a quantum ring* J. Phys.: Condens. Matter **14** (2002) 73
[28a] **B.Szafran**, S.Bednarek, J.Adamowski, *Electric- and magnetic-field-induced evolution of transport windows in a vertical quantum dot* Phys. Rev. B **65** (2002) 35316
[29a] **B.Szafran**, S.Bednarek, J.Adamowski *Magnetic-field-induced transformations of Wigner molecule symmetry in quantum dots* Phys. Rev. B **67** (2003) 045311
[30a] **B.Szafran**, S.Bednarek, J.Adamowski *Correlation effects in vertical quantum dots* Phys. Rev. B **67** (2003) in print.

Dr. Bartlomiej Szafran was involved in three **funded projects** of the Polish State Committee for Scientific Research (KBN):

(1) 1997-1999 Study of the properties of electron and donor states in semiconductor nanostructures. Grant No. 2P03B 5613.
(2) 1999-2000 Study of the electronic properties of semiconductor quantum dots. Grant No. 2P03B 3416.
(3) 2001-2003 Study of the electronic properties of artificial atoms and molecules. Grant No. 2P03B 4920.

Dr. Bartlomiej Szafran participated in the POLONIUM program of French-Polish scientific coopearation between the group of prof. Janusz Adamowski (Kraków, Poland) and of prof. Bernard Stebe (Metz,France). Grant No PL 0502-II/1999/2001(A) “Theory of artificial atoms and exciton complexes in semiconductor nanostructures with reduced dimensionality”).

Curriculum vitae

Bartłomiej Szafran
Faculty of Physics and Nuclear Techniques
University of Mining and Metallurgy (AGH)
Mickiewicza 30, 30-059 Kraków, Poland email: bszafran@agh.edu.pl

Born		06.12.1972 in Stalowa Wola (Poland)
Education	1991-1996:	Master in Computational Physics at the Faculty of Physics & Nuclear Techniques University of Mining and Metallurgy (AGH) Kraków, Poland.
	1995-1996:	Master (DEA) in Physics and Physical Chemistry of the Matter and Materials Metz University, France [Tempus Scholarship].
	1996-2000:	PhD studies in the Faculty of Physics & Nuclear Techniques in Kraków (Poland) and Institute of Physics in Metz (France) [scholarship of the French government], under joint direction (*cotutelle*) of prof. Janusz Adamowski and prof. Bernard Stébé. Title of the thesis: "Electron and donor systems in semiconductor quantum dots". Thesis was awared with distinction on the Polish side and the highest French note [très honorable avec felicitations du jury].
Employment	2000+	permanent researcher in the group of prof. Janusz Adamowski and Stanislaw Bednarek at the Faculty of Physics & Nuclear Techniques, University of Mining and Metallurgy (AGH) Kraków, Poland
		september 2001: invited professor at the University of Metz
Scientific interest		Theory of semiconductor quantum dots, electronic properties, artificial atoms and molecules, Wigner molecules, neutral and charged excitons.
Awards		1999, 2001 – Award of the Minister of Education for the teamwork 2001 – Prime Minister Award for the thesis (granted to about 30 PhDs each year, irrespective of the field) 2001, 2002 – Scholarship of the Foundation for Polish Science attributed to the most promising young researchers.
Other		C and Fortran programmer, fluent in English and French, experience in teaching computational physics and quantum mechanics. Permanent referee of Physical Review Letters, Physical Review B, Physica Status Solidi and Nanotechnology.

B5. Management and feasibility

The project will be realized according to the following work plan:

Month 1: Training in the MC techniques developed in Antwerp. The applicant will apply the MC techniques to the optimization of the centers of the one-electron wave functions in cooperation with Minghui Kong, Bart Partoens and François Peeters [Minghui Kong, B. Partoens, and F.M. Peeters, Phys. Rev. E **65**, 046602].

Month 2: The applicant will work on the optimization of the Hartree-Fock method for the range of the magnetic fields in which the MDD decays. The results of the Hartee-Fock high-magnetic field approach will be compared to the results of the exact diagonalization method for low-magnetic fields developed in Antwerp by Maarten Tavernier. The results of the two-dimensional exact diagonalization scheme of M. Tavernier will be compared to the results of the three-dimensional code developed by the applicant [B. Szafran, S. Bednarek, J.Adamowski Phys. Rev. B **67** 2003, in print].

Month 3: The applicant will study the impact of the solid-solid transitions on the chemical potentials of N electron systems as functions of the external magnetic field. The cusps related to these transformations will be compared with the experimental data [Oosterkamp *et al* Phys. Rev. Lett. **82**, 2931 (1999)].

Month 4. Both the methods used in Month 2 will be applied to structures with nonharmonic confinement potential. The dependence of the ground state configurations of Winger molecules on the strength and profile of the confinement potential will be determined. The applicant will study the electron systems in quantum rings in context of the Wigner crystallization. The results for the phase transition in quantum systems will be compared to the phase transitions in classical systems [I.V. Schweigert, V.A. Schweigert and F.M. Peeters, Phys. Rev. B **54**, 10 827 (1996)].

Month 5: The applicant will develop the exact diagonalization scheme based on mixing of the spatial configuration of Wigner molecules using the multicenter basis. The results will be compared to HF as well as with the exact diagonalization scheme based on low-magnetic field limit developed by M. Tavernier.

Month 6-7: The applicant will be trained in the current spin density functional theory. The code developed by B. Partoens and F.M. Peeters [Europhys. Lett. **56**, 86 (2001)] will be applied to the problem of the decay of the maximum density droplet. The results will be compared to the ones presented in the paper of Reimann *et al.* [Phys. Rev. Lett. **83**, 3270 (1999)].

Month 8-9: The applicant will consider the impact of the random fluctuations of the confinement potential on the Wigner crystallization in large quantum dots. The results will be compared to the experimental data of Zhitenev *et al.* [N.B. Zhitenev *et al.* Phys. Rev. Lett. **79**, 2308 (1997);M. Brodsky *et al.* Phys. Rev. Lett. **85**, 2356 (2000)].

Month 10-11: The applicant will study the problem of the Wigner phases in quantum wires. The study will be performed in cooperation with Giovanni Piacente and Joseph Betouras who work on the quantum wires in Antwerp.

Month 10-12: The applicant will prepare papers on the problems he studied during his stay in Antwerp.

B6. Relevance to the objectives of the activity.

In future the applicant intends to work in Poland, his country of origin. In order to gain the formal professional independence the applicant should prepare a dissertation (equivalent to ancient French *thèse d'état* or German habilitation). This dissertation enables a Polish researcher to direct its own research, to apply for funded projects and to promote PhDs. Dr Szafran prepares his dissertation on the Wigner phase in semiconductor quantum dots. Therefore, the topic of the present proposal is directly connected with the possible achievement of the independence by the researcher. A postdoc position at a good Western university or research institute is a necessary condition for a successful scientific carrier in Poland.

From point of view of the scientific interest of the applicant, the training he needs and his future career, the Antwerp group is an ideal host for a period of mobility and training. Group of prof. Peeters is one of the best European teams in the theoretical physics of semiconductors. In particular, prof. Peeters is one of the pioneers in the study of the Wigner phase in quantum dots, and has an experience of almost a decade of successful work in this field. The Antwerp group studied classical counterpart of the quantum systems which are to be studied in the proposed project, i.e. in the systems of classical point charges confined in quantum dots as well as in quantum rings and quantum wires. The Antwerp group possesses a large experience and expertise in the determination, classification and qualification of such systems. In particular it has developed a set of Monte-Carlo methods for the determination of the configurations of the classical Wigner molecules in various external potentials. Dr Szafran hopes to be able to profit from the expertise of the group of prof. François Peeters in classical Wigner clusters as well as to learn the Monte-Carlo techniques. The applicant has already started working on quantum Wigner molecules and his preliminary achievements are very promising. Namely, dr. Szafran prepared a method of solution of Schroedinger equation, which is able to yield an exact limit of high magnetic field, for which the quantum system resembles its classical counterpart. Moreover, he has shown that in finite magnetic field limit the qualitative properties of quantum system (i.e. the shape of the ground state molecule) are different than in the classical case. The method of treatment of the quantum electron system in Wigner phase developed in Krakow could be combined with the methods for finding the ground and metastable states of classical Wigner molecules created in Antwerp. Namely, the Monte-Carlo techniques developed in Antwerp could be applied to optimize the centers of the one-electron wave functions used in construction of the multicenter basis (c.f. B1). The large experience of prof. Peeters in the field of the proposed project and the recent preliminary achievements of dr. Szafran are complementary and offer an attractive possibility of a fruitful scientific cooperation. A combination of these complementary expertises opens a large area of interesting problems, which could be solved in the cooperation of the Antwerp group with the Krakow group of J. Adamowski. Moreover, they also guarantee that the researchers match the profile of the proposed project.

The HF and exact diagonalization schemes provide a different mechanism of the maximum density droplet decay that the density functional theory (see Part B1.) A comparative study of these methods should be useful in order to understand the physics of the decay. The Antwerp group possesses expertise in DFT. This approach has never been used by the Krakow group, in which the applicant is permanently employed. The applicant should benefit from the mobility period in order to learn the DFT technique and to determine the origin of the differences of the MDD decay mechanisms predicted by HF/exact diagonalization and DFT. This study will be performed in a direct cooperation of the applicant with B. Partoens and F. Peeters. The group of Antwerp possesses expertise in the study of the Wigner crystallization in DFT.

The proposed project lies within a long-term interest of the Antwerp group. On the other hand dr. Szafran will pursue the proposed line of research whether the application is accepted to realization or not, since this line is the subject of the dissertation the preparation of which is under way. A period of mobility and training in Antwerp would make this preparation more efficient, valuable and successful. Dr. Szafran achieved a position of a permanent researcher at his home university in Krakow; therefore he will be able to return safely to his work and duties after the end of the mobility period.

International cooperation is a natural way of making science. Since the Polish science is drastically under financed, the international cooperation is of vital importance for a Polish researcher. A stay at Antwerp, beside the possibility of the training through research, would enable dr. Szafran to gain experience in a work in a large international team. A direct contact with the experimentalists is of invaluable importance for a theoretical physicist. It will be much easier for dr. Szafran to enter in such a contact as a member of the Belgian group, which cooperates with a number of high-quality experimental teams. The realization of the objectives of the project will constitute a significant progress in the state-of-art knowledge in the field, which in its turn will enhance the scientific excellence of EU.

B7. Added value to the Community

The Belgian host and the Polish home team of the applicant possess a complementary expertise and research experience in the field of semiconductor quantum dots. The proposed project deals with the problems of nanotechnology, which is the 3rd priority thematic area of the 6th framework program. The fellowship will enable the groups to start a long-term cooperation, which will enhance the efficiency of both the groups, enable the exchange of knowledge and expertise and to contribute toward formation of the European Research Area. In the past the two groups cooperated in a certain extent. Namely, the group of Krakow took part in the PECO program in 1994/1995 [contract no: erbcipdct940032, coordinator: J. Devreese of Antwerp University]. The cooperation resulted in a common publication [J.M.Shi et al. Phys. Rev. B **57** (1998) 3900]. A more direct cooperation between the groups was hindered by a lack of a young mobile scientist of the Polish group. Dr Szafran has successfully played such a role in 5-years cooperation between the group of J. Adamowski from Krakow and the group of prof. Bernard Stébé of Metz (France). At present the applicant is willing to serve as a link between the Antwerp and Krakow group.

The fellowship will contribute to the development of the research activity in Poland, as one of the associated candidate countries. At present and in the nearest future the scientific researchers in Poland suffer from a lack of funds. However, in the field of theoretical physics the Polish researchers can contribute to the EU scientific excellence, since the research in theoretical physics is cheap. A sad consequence of the poor financial condition of Polish science leads inevitably to the negative selection in the Polish young scientific staff and on its turn to the erosion of the future scientific potential of the country, which will soon be a member of EU. The high quality of the applicant, recognized by several prestigious awards granted in his country of origin (c.f. part B4), is rather an exception to the rule. Therefore, the support of the Marie-Curie Fellowship for dr. Szafran should contribute to the future scientific potential of Poland.

The Antwerp group possesses a well established cooperation with the researchers from countries of Eastern Europe. A personal contact of the applicant with the young researchers from Eastern Europe could be useful in future cooperation between the countries in these part of the continent.