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14. ABSTRACT

We implemented a program of research and education that aims to understand various electronic and spintronic effects that occur in confined two-dimensional semiconductor quantum dot systems. Semiconductor quantum dots represent nanoscale systems made of few confined electrons. Their properties are size-dependent and of great interest to many disciplines. The interplay between quantum confinement, correlation effects, spin, electric and/or magnetic field gives rise to very interesting physical phenomena. We considered new concepts for controlled

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Report Title

Final Report: New Concepts For Controlled Injection, Detection, and Manipulation of Spin in Quantum Dot Devices

ABSTRACT

We implemented a program of research and education that aims to understand various electronic and spintronic effects that occur in confined two-dimensional semiconductor quantum dot systems. Semiconductor quantum dots represent nanoscale systems made of few confined electrons. Their properties are size-dependent and of great interest to many disciplines. The interplay between quantum confinement, correlation effects, spin, electric and/or magnetic field gives rise to very interesting physical phenomena. We considered new concepts for controlled injection, detection and manipulation of spin in various types of quantum dot devices. We investigated novel spintronic devices of high tunability that are built from coupled quantum dot systems of electrons with spin-orbit coupling. We elucidated the role plaid by an electric field on controlling the spin polarization and spin interference effects in confined nanoscale systems of electrons. We also studied the possible existence of novel quantum phases of confined electrons that may arise in presence of a magnetic field as well as the overall influence of size, shape and geometry on the properties of small finite systems of particles. The educational benefits are self-evident from the perspective of an HBCU institution. Participation and involvement of undergraduate students in the research has been very successful.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
07/18/2017	14	Orion Ciftja. Anisotropic quantum Hall liquid states with no translational invariance in the lowest Landau level, Journal of Low Temperature Physics, (08 2015): 85. doi: 365,209.00
07/18/2017	42	Orion Ciftja. Stored Coulomb Self-Energy of a Uniformly Charged Rectangular Plate, Advances in Mathematical Physics, ( ): 1. doi: 1,050,559.00
07/18/2017	40	Josep Batle, Orion Ciftja, Mosayeb Naseri, Mahmood Ghoranneviss, Koji Nagata, Tadao Nakamura. Coulomb self-energy integral of a uniformly charged d-cube: A physically-based method for approximating multiple integrals, Journal of Electrostatics, ( ): 52. doi: 1,050,557.00
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07/18/2017	38	Orion Ciftja. Anisotropic magnetoresistance and piezoelectric effect in GaAs Hall samples, Physical Review B, ( ): . doi: 1,050,553.00
07/18/2017	37	Orion Ciftja, Victoria Livingston, Elsa Thomas. Cyclotron motion of a charged particle with anisotropic mass, American Journal of Physics, ( ): 359. doi: 1,050,552.00
07/18/2017	36	Zhaosen Liu, Orion Ciftja, Hou Ian. Interplay of Dzyaloshinsky-Moriya and dipole-dipole interactions and their joint effects upon vortical structures on nanodisks, Physica E: Low-dimensional Systems and Nanostructures, ( ): 13. doi: 1,050,551.00
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08/13/2014	4	Orion Ciftja. Understanding electronic systems in semiconductor quantum dots, Physica Scripta, (11 2013): 58302. doi: 10.1088/0031-8949/88/05/058302 330,368.00
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08/23/2016	16	Orion Ciftja, Dode Prenga. Magnetic properties of a classical XY spin dimer in a “planar” magnetic field, Journal of Magnetism and Magnetic Materials, ( ): 220. doi: 1,015,041.00
08/23/2016	29	Orion Ciftja; Dode Prenga. Magnetic properties of a classical XY spin dimer in a “planar” magnetic field, Journal of Magnetism and Magnetic Materials, ( ): . doi: 1,015,090.00
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08/23/2016	20	Orion Ciftja. Electric field controlled spin interference in a system with Rashba spin-orbit coupling, AIP Advances, ( ): 055217. doi: 1,015,048.00
08/23/2016	21	Orion Ciftja. Anisotropic Quantum Hall Liquid States with No Translational Invariance in the Lowest Landau Level, Journal of Low Temperature Physics, ( ): 85. doi: 1,015,051.00
08/24/2016	30	Orion Ciftja ; Victoria Livingston ; Elsa Thomas. Cyclotron motion of a charged particle with constant anisotropic mass, American Journal of Physics, ( ): . doi: 1,015,186.00
08/24/2016	31	Orion Ciftja. Anisotropic magneto-resistance and piezoelectric effect in GaAs Hall samples, Physical Review B, ( ): . doi: 1,015,187.00
08/27/2015	5	Orion Ciftja. Hartree–Fock energy of a finite two-dimensional electron gas system in a jellium background, Physica B: Condensed Matter, (02 2015): 92. doi: 10.1016/j.physb.2014.11.019 365,172.00
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08/27/2015	10	Orion Ciftja. Quantitative analysis of shape-sensitive interaction of a charged nanoplate and a charged nanowire, Nano, (07 2015): 1550114. doi: 10.1142/S1793292015501143 365,180.00
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Number of Papers published in peer-reviewed journals:

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Received	Paper

TOTAL: 2

Number of Papers published in non peer-reviewed journals:

(c) Presentations

V. Livingston*, E. Thomas*, S. Saganti*, and O. Ciftja, Anisotropic magneto-resistance and piezoelectric effect in GaAs Hall samples, 2016 Joint MMM-Intermag Conference, San Diego, California, USA, January 11-15, 2016.

O. Ciftja, Electric field controlled spin interference in a system with Rashba spin-orbit coupling, 2016 Joint MMM-Intermag Conference, San Diego, California, USA, January 11-15, 2016.

O. Ciftja, V. Livingston*, E. Thomas*, and S. Saganti*, Finite two-dimensional electron gas in a patterned semiconductor system, APS March Meeting 2016, Baltimore, Maryland, USA, March 14-18, 2016.

O. Ciftja, Magnetoresistance Anisotropy of a Two-Dimensional Electron System on a GaAs Substrate, 2016 MRS Conference, Phoenix, Arizona, USA, March 29 – April 1, 2016.

O. Ciftja, Anisotropic Electronic States In The Fractional Quantum Hall Regime,61st Annual Conference on Magnetism and Magnetic Materials (MMM), New Orleans, LA, USA, October 31-November 4, 2016.

Elsa Thomas*, Seth Saganti* and Orion Ciftja, Size-dependent energy of a confined system of two-dimensional electrons, 13th TAMUS Pathways Conference, November 3-4, 2016.

Number of Presentations: 6.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received		Paper
07/18/2017	45	Orion Ciftja. Anisotropic electronic states in the fractional quantum Hall regime, 61st Conference on Magnetism and Magnetic Materials (MMM). 31-OCT-16, New Orleans, LA, USA. : ,
08/23/2016	26	Orion Ciftja. Anisotropic quantum Hall liquid states with no translational invariance in the lowest Landau level, International Symposium on Quantum Fluids and Solids. 09-JUL-15, Niagara Falls, NY. : ,

TOTAL: 2

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received   Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received   Paper

TOTAL:

Number of Manuscripts:

Books

Received   Book

08/24/2016 3.00 Arjan Ciftja ; Orion Ciftja. Energy Technology 2014, Hoboken, NJ, USA: John Wiley & Sons, Inc., (02 2014)

TOTAL: **1**

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Student Presentation [E. Thomas, S. Saganti, and O. Ciftja, Size-dependent energy of a confined system of two-dimensional electrons] won Poster award in the 13th TAMUS Pathways Conference, November 3-4, 2016.

Graduate Students

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FTE Equivalent:
Total Number:

Names of Post Doctorates

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FTE Equivalent:
Total Number:

Names of Faculty Supported

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Total Number:

Names of Under Graduate students supported

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Student Metrics

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This section can include, but is not limited to:

(1) Foreword (optional)

The Principal Investigator (PI) of this award established a strong integrated program of research and education that dealt with spintronic effects in two-dimensional semiconductor quantum dots. The PI used this research opportunity to involve undergraduate students in research as well as educational activities. This resulted in better engagement of underrepresented minorities towards the goal of pursuing careers in science. The proposed research program focused on the theory and modeling of spin effects in two-dimensional semiconductor quantum dots. The results obtained by using a combination of theoretical and state-of-the-art modeling methods improved our understanding of spin effects at different length scales and regimes. The main research objectives were to: (i) Investigate novel spintronic devices of high tunability built from few electron quantum dots where controlled manipulation of electron’s spin is done via an electric field; (ii) Study the theoretical applicability of a sensitive state/spin quantum measurement scheme (via Berry phases) for electrons in a quantum dot; (iii) Characterize various electronic phases of large systems of electrons in zero magnetic field; (iv) Study the influence of confinement on the properties of low-dimensional electron systems; and (v) Study the impact of magnetic field on the spin polarization and stability of various quantum Hall phases of electrons.

(2) Table of Contents (if report is more than 10 pages)

N/A

(3) List of Appendixes, Illustrations and Tables (if applicable)

N/A

(4) Statement of the problem studied

There have been intense research efforts over the last years focused on understanding the Rashba spin-orbit coupling effect in two-dimensional systems of electrons hosted in semiconductor structures that lack inversion symmetry. An important component of this line of research is aimed at control and manipulation of electron’s spin degrees of freedom in semiconductor quantum dot devices. The Rashba spin-orbit coupling effect may potentially lead to fabrication of a new generation of spintronic devices where control of spin, thus control of magnetic properties, is achieved via an electric field. We studied two specific topics within this framework:

A) Feasibility of spintronic devices where spin interference effects in a Rashba spin-orbit coupled system of quantum dots leads to reliable spin control via an electric field; and

B) Properties of spin-orbit coupled systems where the dominant interaction is the Dzyaloshinsky-Moriya (DM) mechanism (ultimately related to the spin-orbit coupling effect).

The behavior of confined low-dimensional electron systems with or without an applied magnetic field is both fascinating and challenging. The interplay between several factors gives rise to many possible scenarios that are not easy to predict or control. In quantum systems, the energy spectrum of a particle is determined by the nature of the confinement potential. To this effect, we deemed important to understand the role played by confinement in small low-dimensional finite systems with a small number of particles. The key topic studied in this context was:

C) Properties of a finite one-dimensional electron gas (1DEG) or two-dimensional electron gas (2DEG) model under various geometries.

Recent experiments in two-dimensional electron systems in a perpendicular magnetic field have indicated the presence of new anisotropic quantum Hall states at regimes not anticipated before. These experiments raise many fundamental questions regarding the inner nature of the electronic system that leads to such anisotropic states. The interplay between structural anisotropy, electron mass anisotropy and electron-electron correlation effects can create a rich variety of possibilities in a magnetic field. The combination of so many factors may lead to the stabilization of novel quantum phases of electrons with unconventional properties. We have studied two specific topics within this framework:

D) Anisotropic behavior in low-dimensional systems and/or anisotropic quantum Hall-like phases of electrons; and

E) Role of finite size, confinement and geometry on various properties of nano-systems.

(5) Summary of the most important results

A) Feasibility of spintronic devices where spin interference effects in a Rashba spin-orbit coupled system of quantum dots lead to reliable spin control via an electric field:

We introduced and investigated a spintronic device that would operate based on the electron's spin interference and accumulation process in a Rashba spin-orbit coupled system consisting of a pair of two-dimensional semiconductor quantum dots connected to each other via two conducting semi-circular channels [14]. The strength of the confinement energy on the quantum dots is tuned by gate potentials that allow "leakage" of electrons from one dot to another. The electron's spin experiences a spin-orbit coupling with a microscopically generated electric field applied perpendicular to the two-dimensional system while going through the conducting channels. We showed that interference of spin wave functions of the electrons travelling through the two channels gives rise to interference/conductance patterns that lead to the observation of the geometric Berry's phase. Achieving a predictable and measurable observation of Berry's phase allows us to control the spin dynamics of the electrons. It is demonstrated that this system allows use of a microscopically generated electric field to control Berry's phase, thus, enables us to tune the spin-dependent interference pattern and spintronic properties with no need for injection of spin-polarized electrons.

We studied in great detail the electronic and spintronic properties of two-dimensional (2D) semiconductor quantum dot nanostructures. Such nanostructures are fabricated by patterning a two-dimensional electron gas (2DEG) created at the interface of a semiconductor heterojunction/heterostructure. Properties of confined electron systems in a 2D semiconductor quantum dot depend on several length scales and energy scales. Our results provided a detailed description of such parameters for a specific model and we also calculated such values for typical experimental situations [26]. Since there are many different forms of confinement felt by electrons, we also studied in detail some of the most popular models that describe the quantum confinement effects in a 2D semiconductor quantum dot. The interplay between quantum confinement, electron-electron correlation effects and magnetic field gives rise to more complicated phenomena as illustrated by various quantum regimes that may arise in a 2D semiconductor quantum dot system. In particular, we studied the theoretical feasibility of various spin-based devices built from 2D semiconductor quantum dot systems. Our results indicate that there are several possible schematic spintronic devices that would serve as a nanoscale prototype to manipulate spin by means of an electric field [14, 26]. These results have many ramifications in the field of spintronics from both a theoretical and an experimental perspective.

Clusters of cold systems of particles under confinement drew our attention when we became aware that there are many "magnetic", thus "spintronic" effects that can be simulated in a Bose-Einstein condensate. In particular, rapidly rotating two-dimensional ultra-cold Bose-Einstein condensates of bosons in a harmonic trap have attracted a considerable interest during the recent years. It turns out that rotation of such systems around the direction perpendicular to the plane effectively leads to a perpendicular "magnetic" field (which in turn couples to the spin). It is expected that in the fast-rotation limit, the system of bosons will exhibit collective behavior analogous to that of two-dimensional electrons in the fractional quantum Hall effect regime of a strong "magnetic" field. Furthermore, there are predictions that the most robust correlated bosonic state in this regime will be a Bose Laughlin state. Our results showed that a transformation to Jacobi coordinates allows us to obtain much desirable exact analytic closed-form expressions for various quantities corresponding to a Bose Laughlin wave function for some finite systems of particles [24]. These results can be directly compared to experimental findings for small systems of rotating particles under a harmonic confinement potential. We believe that the results we report would be of great interest to the specialized, as well as to the broad audience of researchers working in the field of ultra-cold atomic gases.

Doped dilute magnetic oxides such as ZrO2, ZnO, or similar semiconducting oxides have been known to have possible applications in the field of spintronic semiconductor devices. Semiconducting materials of this nature are typically doped with transition-metals such as Co or Mn in order to improve their magnetic properties. Low-dimensional samples of these materials (for instance, thin films) mirror some of the theoretical phenomena [25] that we anticipate should happen in a 2D semiconductor quantum dot system. To this effect, the PI carried out some collaborative work to conduct experiments on certain thin films (confined two-dimensional systems) that manifest interesting magnetic (spintronic) cooperative behavior. We studied the structural and magnetic properties of Al-Mn-doped ZrO2 and ZnO thin films. It was found that co-doping with Al does not enhance the magnetization of Mn-doped ZrO2 samples. However, it was noticed that co-doping with Al results in an enhancement of surface magnetism. On the other hand, it was found that co-doping with Al of Mn-doped ZnO samples results in a significant increase of the magnetic moment. These results confirm that co-doping with Al can be an efficient tool to enhance magnetism (with possible spintronic applications) and control the distribution of defects who play a major role in certain classes of transition-metal-doped semiconducting oxides [23].

B) Properties of spin-orbit coupled systems where the dominant interaction is the Dzyaloshinsky-Moriya (DM) mechanism (ultimately related to the spin-orbit coupling effect):

We investigated the properties of spin-orbit coupled systems in nano-disks where the dominant interaction is the Dzyaloshinsky-Moriya (DM) mechanism. Spin simulations of this nature are extremely difficult. Thus, we first tested a newly developed quantum simulation method by using it to study the properties of a three-dimensional (3D) Ising model consisting of S = 1/2 quantum spins localized at the sites of a simple cubic lattice [4]. We assumed nearest-neighbor interaction between spins with an exchange interaction that can be either ferromagnetic or antiferromagnetic. It was found that the computational method quickly converges towards the expected equilibrium spin configurations. The resulting spontaneous magnetization curves corresponding to the two types of magnetic interactions under consideration were found to be almost identical to the ones obtained via quantum mean field theory at all temperatures. The derived total energies, total free energies, magnetic entropies and specific heats per mole of spins show no sizeable differences from known theoretical values. Furthermore, the results of the simulations for two different 3D Ising systems containing 4x4x4 and 20x20x20 spins localized at the sites of a simple cubic lattice were found to be almost identical to each other. This finding suggests that the self-consistent algorithm approach of the current simulation method allows one to obtain the physical bulk properties of a large magnetic system by relying on simulations of a much smaller spin system sample. Therefore, the method presently considered appears to be not only very accurate as gauged by comparison to mean field theory, but also able to greatly increase the speed of simulations to be used for more complex spin systems.

After having gained confidence on the computational aspects of the approach, we applied the method to study DM coupled spins in nano-disk systems. It happens that the magnetic dipole-dipole (DD) and the chiral DM interactions between nearest neighboring spins are comparable in magnitude in transition metal oxides. In particular, the effects of the DD interaction on the physical properties of magnetic nanosystems cannot be simply neglected due to its long-range character. For these reasons, we investigated the interplay of these two interactions and studied their combined effects upon the magnetic vortical structures of monolayer nanodisks [5]. We found out from our computational results that, in the presence of Heisenberg exchange interaction, a sufficiently strong DD interaction is able to induce a single magnetic vortex on a small nanodisk. A strong DM interaction usually gives rise to a multi-domain structure which evolves as a function of the temperature. In this circumstance, if a weak DD interaction is further considered, the multi-domains merge to form a single vortex in the whole magnetic phase. It was noted that, if only the Heisenberg exchange and chiral DM interactions are considered in simulations, the transition temperature is simply proportional to the size of the total spin (squared).

C) Properties of a finite one-dimensional electron gas (1DEG) or two-dimensional electron gas (2DEG) model under various geometries.

We studied the properties of small quantum Hall systems of electrons in a finite square geometry for a standard Coulomb interaction potential between particles. We adopted the Landau gauge which is the suitable one for a square geometry. We calculated all quantities of interest that correspond to systems with an arbitrary number of particles. In order to involve undergraduate students in meaningful research, we also "simplified" the problem to a semi-classical model that the undergraduate students would understand better. The basic idea was to treat the electrons not as point-like particles, but as extended 1D "rod-like/stripe" objects [1] with their charge uniformly spread (this treatment is plausible for the case of electrons moving in 2D in presence of a perpendicular magnetic field when the Landau gauge is used). In such a case, we obtained the precise form of the effective/modified interaction potential between the resulting "rod-like/stripe" structures in an elongated quasi-1D system [22]. This model is also important to mathematical physics studies as well as biological systems that routinely deal with elongated "rod-like/stripe" structures.

We calculated various properties of a finite one-dimensional electron gas (1DEG) model for any given arbitrary number of particles [21]. The homogeneous electron gas model has been quite successful to predict the bulk properties of systems of electrons at various densities. In many occasions, a simplified free homogeneous electron gas model represents a powerful first approximation to a real system. Despite our considerable knowledge on the bulk properties of a homogeneous electron gas, advances in nanoscience and nanotechnology call for a greater effort to understand the opposite limit of small finite systems of electrons with size-dependent properties. We provided a detailed description of the properties of a finite fully spin-polarized (spinless) free homogeneous 1DEG. We derived exact analytical results for various quantities such as the one-particle density function, two-particle density function, one-particle density matrix, pair correlation function and energy of finite systems with an arbitrary number of electrons.

We calculated the energy and various properties of a finite two-dimensional electron gas (2DEG) model [20]. We found some very interesting non-monotonic variations of the energy of the system when the finite number of electrons changes value. We adopted a Hartree-Fock approach and calculated the energy of a finite 2DEG system confined to a region that is treated as a positive jellium background. The electrons are considered fully spin-polarized (spinless) and interact with a Coulomb potential. The calculation of the exact potential energy of electrons in a finite square jellium domain is very challenging since the mathematical expressions depend in each component of particle's position and not the radial distance from the center of the domain. In order to address this issue we introduced an approximation to the problem. We assessed the quality of this approximation and discussed instances where its use is not only desirable, but also fairly accurate. The results give a correct picture of how the energy of the finite system evolves towards the bulk value as the size of the system increases.

D) Anisotropic behavior in low-dimensional systems and/or anisotropic quantum Hall-like phases of electrons:

We investigated anisotropic behavior in low-dimensional systems and/or anisotropic quantum Hall-like phases of electrons from the perspective of liquid crystalline phases. In our view, the source of anisotropy in certain quantum Hall systems (with GaAs as a host) is the piezo-electric effect that comes from the host substrate [7]. The piezo-electric effect effectively leads to an anisotropic interaction between electrons (a similar effect is also attributed to an effective anisotropic mass). An anisotropic interaction potential may strongly influence the stability of various quantum phases that are close in energy since the overall stability of an electronic system is very sensitive to local order. As a result, there is possibility that various anisotropic electronic phases may emerge even in the lowest Landau level in regimes where one would not expect them. We studied the state with filling factor 1/6 in the lowest Landau level. This state is very close to the critical filling factor where the liquid-solid transition takes place. We investigated whether an anisotropic Coulomb interaction potential is able to stabilize an anisotropic electronic liquid state at this filling factor. We described such an anisotropic state by means of a liquid crystalline wave function with broken rotational symmetry which can be adiabatically connected to the actual wave function for the corresponding isotropic phase. We performed quantum Monte Carlo simulations in a disk geometry [3] to study the properties of the anisotropic electronic liquid state under consideration. The findings [8] indicate stability of liquid crystalline order in presence of an anisotropic Coulomb interaction potential. The results are consistent with the existence of an anisotropic electronic liquid state in the lowest Landau level.

We take the opportunity to remark that certain aspects of this research were also well suited to the level of preparation of undergraduate students. Undergraduate students were actively engaged in all phases of the project. In particular, they worked on a study that dealt with the concept of anisotropic mass. Their efforts ultimately led to a publication of a peer-reviewed paper [6]. The focus was on the cyclotron motion of a charged particle subject to a uniform magnetic field which is thoroughly described in many classical physics textbooks. Although the assumption of a particle with isotropic mass is taken for granted in classical physics, a key concept in condensed matter physics is that of particles that have an effective anisotropic mass such as electrons in the context of band structure studies of solids. Since some exposure to the concept of anisotropic mass is important within the framework of classical physics, we considered the cyclotron motion of a charged particle with anisotropic mass in the presence of a uniform magnetic field. The exact solution of this problem exposes a broad audience of readers to concepts in condensed matter physics that are rarely mentioned within the framework of classical physics. Key ideas on the topic were illustrated in a pedagogical way by considering specific examples that show how an anisotropic mass modifies the cyclotron motion of a charged particle.

We completed a detailed study of the properties of a specific class of anisotropic quantum Hall liquid states of electrons that lack translational invariance [15]. We used a novel class of anisotropic Fermi wave functions to this effect. We used this approach to explain recent unanticipated findings that indicate the presence of an anisotropic fractional quantum Hall state in the lowest Landau level. The key expectation of our work was that novel anisotropic liquid phases of electrons may stabilize even in a strong magnetic field regime where normally one expects to see only isotropic quantum Hall liquid states. Although the energy of the anisotropic wave function under consideration was somehow higher than the energy of the competing uniform isotropic liquid phases, we still believe that additional refinements of the approach may ultimately lead to more interesting results.

E) Role of finite size, confinement and geometry on various properties of nano-systems:

The research in this direction spanned several topics such as: (i) Confined two-dimensional electronic systems under various geometries; (ii) Confined spin-polarized fermion systems in the quantum regime; and (iii) Models of nano-structures and/or finite systems with various geometries and shapes.

(i) We studied the minimum energy equilibrium configurations of a classical two-dimensional system of point charges confined by a triangular, square and disk region with a hard-wall boundary [10]. It is assumed that the point charges interact via a repulsive Coulomb interaction potential. Monte Carlo simulations with the annealing algorithm suggest that the equilibrium configurations of a given system are strongly influenced by the external (isotropic/anisotropic) geometry of the hard-wall boundary. The numerically obtained energies extrapolated in the bulk limit converge to the expected continuum equilibrium values (when known). It is found that the equilibrium charge distribution is non-uniform in the continuum limit for all the hard-wall confining regions considered. Since the continuum equilibrium charge distribution is not known for the case of an equilateral triangle or a square domain we choose to compare the numerically obtained bulk energy results to corresponding values for a uniformly charged system [9, 17]. We calculated exactly the electrostatic energy of various uniformly charged planar objects and used the findings to assess the discrepancy between such results and the numerically obtained equilibrium bulk energy values for the cases of an equilateral triangle and a square hard-wall boundary. These estimates help us understand how an anisotropic boundary with the shape of an equilateral triangle or square influences the energy of an equilibrium charge distribution. The results indicate that the energy discrepancy between equilibrium and uniform charge distributions in the continuum limit is not very large. It is found that the order of magnitude of the relative deviation of the energy for all three different planar domains considered here is approximately the same.

(ii) There have been suggestions that the Pauli's exclusion principle alone can lead a non-interacting (free) system of identical fermions to form crystalline structures dubbed Pauli crystals. Single-shot imaging experiments for the case of ultra-cold systems of free spin-polarized fermionic atoms in a two-dimensional harmonic trap appear to show geometric arrangements that cannot be characterized as Wigner crystals. We explored this rather exotic idea. We considered a well-known approach that enables one to treat a quantum system of free fermions as a system of classical particles interacting with a statistical interaction potential. The model under consideration, though classical in nature, incorporates the quantum statistics by endowing the classical particles with an effective interaction potential. The reasonable expectation is that possible Pauli crystal features (claimed to have been seen in experiments) may manifest in this model that captures the correct quantum statistics as a first order correction. We use the Monte Carlo simulated annealing method to obtain the most stable configurations of finite two-dimensional systems of confined particles that interact with an appropriate statistical repulsion potential [2]. We consider both an isotropic harmonic and a hard-wall confinement potential. Despite minor differences, the most stable configurations observed in our model correspond to the reported Pauli crystals in single-shot imaging experiments of free spin polarized fermions in a harmonic trap. The crystalline configurations observed appear to be different from the expected classical Wigner crystal structures that would emerge should the confined classical particles had interacted with a pair-wise Coulomb repulsion. This result might likely represent the first theoretical confirmation (in broad features) of this very strange idea (though, we caution that one must be very careful and reserved with regard to the existence or not of Pauli crystals).

(iii) We achieved a good understanding of how geometry/shape/etc. influences the properties of small finite systems of electrons at the nanoscale by considering several models. We believe that finite systems (with small number of particles) constitute a good starting point to get an understanding of bulk effects. Such systems also serve as a good starting basis to engage undergraduate students into research. The external confining geometry, shape of the confining region, nature of the host material, microscopic nature of the interaction potentials, etc. influences the properties of small finite systems of electrons. In order to gain insight of how finite size, confinement and geometry influences/enhances anisotropic features in small finite systems of particles, we calculated various shape-sensitive interaction potentials [11, 12, 16]. The results obtained are useful to calculate the properties of small systems of electrons confined in nanoscale domains. The acquisition of such a knowledge can be useful to extend the treatment to larger structures containing electrons. In many cases, the overall properties of low-dimensional strongly correlated electronic systems depend crucially on the spin of the electrons. Calculation of spin properties is difficult even for simple models [13]. In order to understand the impact that geometry/shape has on the properties of a finite 2DEG system, the PI together with undergraduate students calculated the shape-dependent energy for a 2D elliptical jellium system [18]. This result will be very useful to calculate the energy of a distorted 2DEG with elliptical Fermi surface, a system that is believed to exist under certain conditions.

(6) Bibliography

The best measurable outcome of research productivity is the number of peer-reviewed papers published by the PI and his collaborators. Below is a complete list of peer-reviewed papers published with support from this grant during the last 3-4 years.

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(7) Appendixes

N/A

Technology Transfer

The PI made a presentation of his work on spintronic devices during the Industry Day exhibition at Prairie View A&M University on April 27, 2016. At the time, the PI had some interaction and exchange of ideas with industry partners. The PI discussed possible technology transfer and/or patenting of ideas at the time.

Scientific Progress and Accomplishments

(Description should include significant theoretical or experimental advances) Plain Text Only - If you have diagrams, formula's, etc. in a Word, PDF or other document, enter "See Attachment" below and use the "Attachment" section at the bottom of the menu.

This section can include, but is not limited to:

(1) Foreword (optional)

The Principal Investigator (PI) of this award established a strong integrated program of research and education that dealt with spintronic effects in two-dimensional semiconductor quantum dots. The PI used this research opportunity to involve undergraduate students in research as well as educational activities. This resulted in better engagement of underrepresented minorities towards the goal of pursuing careers in science. The proposed research program focused on the theory and modeling of spin effects in two-dimensional semiconductor quantum dots. The results obtained by using a combination of theoretical and state-of-the-art modeling methods improved our understanding of spin effects at different length scales and regimes. The main research objectives were to**: (i)** Investigate novel spintronic devices of high tunability built from few electron quantum dots where controlled manipulation of electron's spin is done via an electric field; **(ii)** Study the theoretical applicability of a sensitive state/spin quantum measurement scheme (via Berry phases) for electrons in a quantum dot**; (iii)** Characterize various electronic phases of large systems of electrons in zero magnetic field; **(iv)** Study the influence of confinement on the properties of low-dimensional electron systems; and **(v)** Study the impact of magnetic field on the spin polarization and stability of various quantum Hall phases of electrons.

(2) Table of Contents (if report is more than 10 pages)

N/A

(3) List of Appendixes, Illustrations and Tables (if applicable)

N/A

(4) Statement of the problem studied

There have been intense research efforts over the last years focused on understanding the Rashba spin-orbit coupling effect in two-dimensional systems of electrons hosted in semiconductor structures that lack inversion symmetry. An important component of this line of research is aimed at control and manipulation of electron's spin degrees of freedom in semiconductor quantum dot devices. The Rashba spin-orbit coupling effect may potentially lead to fabrication of a new generation of spintronic devices where control of spin, thus control of magnetic properties, is achieved via an electric field. We studied two specific topics within this framework:

A) Feasibility of spintronic devices where spin interference effects in a Rashba spin-orbit coupled system of quantum dots leads to reliable spin control via an electric field; and

B) Properties of spin-orbit coupled systems where the dominant interaction is the Dzyaloshinsky-Moriya (DM) mechanism (ultimately related to the spin-orbit coupling effect).

The behavior of confined low-dimensional electron systems with or without an applied magnetic field is both fascinating and challenging. The interplay between several factors gives rise to many possible scenarios that are not easy to predict or control. In quantum systems, the energy spectrum of a particle is determined by the nature of the confinement potential. To this effect, we deemed important to understand the role played by confinement in small low-dimensional finite systems with a small number of particles. The key topic studied in this context was:

C) Properties of a finite one-dimensional electron gas (1DEG) or two-dimensional electron gas (2DEG) model under various geometries.

Recent experiments in two-dimensional electron systems in a perpendicular magnetic field have indicated the presence of new anisotropic quantum Hall states at regimes not anticipated before. These experiments raise many fundamental questions regarding the inner nature of the electronic system that leads to such anisotropic states. The interplay between structural anisotropy, electron mass anisotropy and electron-electron correlation effects can create a rich variety of possibilities in a magnetic field. The combination of so many factors may lead to the stabilization of novel quantum phases of electrons with unconventional properties. We have studied two specific topics within this framework:

D) Anisotropic behavior in low-dimensional systems and/or anisotropic quantum Hall-like phases of electrons; and

E) Role of finite size, confinement and geometry on various properties of nano-systems.

(5) Summary of the most important results

A) Feasibility of spintronic devices where spin interference effects in a Rashba spin-orbit coupled system of quantum dots lead to reliable spin control via an electric field:

We introduced and investigated a spintronic device that would operate based on the electron's spin interference and accumulation process in a Rashba spin-orbit coupled system consisting of a pair of two-dimensional semiconductor quantum dots connected to each other via two conducting semi-circular channels [14]. The strength of the confinement energy on the quantum dots is tuned by gate potentials that allow “leakage” of electrons from one dot to another. The electron’s spin experiences a spin-orbit coupling with a microscopically generated electric field applied perpendicular to the two-dimensional system while going through the conducting channels. We showed that interference of spin wave functions of the electrons travelling through the two channels gives rise to interference/conductance patterns that lead to the observation of the geometric Berry’s phase. Achieving a predictable and measurable observation of Berry’s phase allows us to control the spin dynamics of the electrons. It is demonstrated that this system allows use of a microscopically generated electric field to control Berry’s phase, thus, enables us to tune the spin-dependent interference pattern and spintronic properties with no need for injection of spin-polarized electrons.

We studied in great detail the electronic and spintronic properties of two-dimensional (2D) semiconductor quantum dot nanostructures. Such nanostructures are fabricated by patterning a two-dimensional electron gas (2DEG) created at the interface of a semiconductor heterojunction/heterostructure. Properties of confined electron systems in a 2D semiconductor quantum dot depend on several length scales and energy scales. Our results provided a detailed description of such parameters for a specific model and we also calculated such values for typical experimental situations [26]. Since there are many different forms of confinement felt by electrons, we also studied in detail some of the most popular models that describe the quantum confinement effects in a 2D semiconductor quantum dot. The interplay between quantum confinement, electron-electron correlation effects and magnetic field gives rise to more complicated phenomena as illustrated by various quantum regimes that may arise in a 2D semiconductor quantum dot system. In particular, we studied the theoretical feasibility of various spin-based devices built from 2D semiconductor quantum dot systems. Our results indicate that there are several possible schematic spintronic devices that would serve as a nanoscale prototype to manipulate spin by means of an electric field [14, 26]. These results have many ramifications in the field of spintronics from both a theoretical and an experimental perspective.

Clusters of cold systems of particles under confinement drew our attention when we became aware that there are many "magnetic", thus "spintronic" effects that can be simulated in a Bose-Einstein condensate. In particular, rapidly rotating two-dimensional ultra-cold Bose-Einstein condensates of bosons in a harmonic trap have attracted a considerable interest during the recent years. It turns out that rotation of such systems around the direction perpendicular to the plane effectively leads to a perpendicular "magnetic" field (which in turn couples to the spin). It is expected that in the fast-rotation limit, the system of bosons will exhibit collective behavior analogous to that of two-dimensional electrons in the fractional quantum Hall effect regime of a strong "magnetic" field. Furthermore, there are predictions that the most robust correlated bosonic state in this regime will be a Bose Laughlin state. Our results showed that a transformation to Jacobi coordinates allows us to obtain much desirable exact analytic closed-form expressions for various quantities corresponding to a Bose Laughlin wave function for some finite systems of particles [24]. These results can be directly compared to experimental findings for small systems of rotating particles under a harmonic confinement potential. We believe that the results we report would be of great interest to the specialized, as well as to the broad audience of researchers working in the field of ultra-cold atomic gases.

Doped dilute magnetic oxides such as ZrO_2, ZnO, or similar semiconducting oxides have been known to have possible applications in the field of spintronic semiconductor devices. Semiconducting materials of this nature are typically doped with transition-metals such as Co or Mn in order to improve their magnetic properties. Low-dimensional samples of these materials (for instance, thin films) mirror some of the theoretical phenomena [25] that we anticipate should happen in a 2D semiconductor quantum dot system. To this effect, the PI carried out some collaborative work to conduct experiments on certain thin films (confined two-dimensional systems) that manifest interesting magnetic (spintronic) cooperative behavior. We studied the structural and magnetic properties of Al-Mn-doped ZrO_2 and ZnO thin films. It was found that co-doping with Al does not enhance the magnetization of Mn-doped ZrO_2 samples. However, it was noticed that co-doping with Al results in an enhancement of surface magnetism. On the other hand, it was found that co-doping with Al of Mn-doped ZnO samples results in a significant increase of the magnetic moment. These results confirm that co-doping with Al can be an efficient tool to enhance magnetism (with possible spintronic applications) and control the distribution of defects who play a major role in certain classes of transition-metal-doped semiconducting oxides [23].

B) <u>Properties of spin-orbit coupled systems where the dominant interaction is the Dzyaloshinsky-Moriya (DM) mechanism (ultimately related to the spin-orbit coupling effect):</u>

We investigated the properties of spin-orbit coupled systems in nano-disks where the dominant interaction is the Dzyaloshinsky-Moriya (DM) mechanism. Spin simulations of this nature are extremely difficult. Thus, we first tested a newly developed quantum simulation method by using it to study the properties of a three-dimensional (3D) Ising model consisting of $S = 1/2$ quantum spins localized at the sites of a simple cubic lattice [4]. We assumed nearest-neighbor interaction between spins with an exchange interaction that can be either ferromagnetic or antiferromagnetic. It was found that the computational method quickly converges towards the expected equilibrium spin configurations. The resulting spontaneous magnetization curves corresponding to the two types of magnetic interactions under consideration were found to be almost identical to the ones obtained via quantum mean field theory at all temperatures. The derived total energies, total free energies, magnetic entropies and specific heats per mole of spins show no sizeable differences from known theoretical values. Furthermore, the results of the simulations for two different 3D Ising systems containing 4x4x4 and 20x20x20 spins localized at the sites of a simple cubic lattice were found to be almost identical to each other. This finding suggests that the self-consistent algorithm approach of the current simulation method allows one to obtain the physical bulk properties of a large magnetic system by relying on simulations of a much smaller spin system sample. Therefore, the method presently considered appears to be not only very accurate as gauged by comparison to mean field theory, but also able to greatly increase the speed of simulations to be used for more complex spin systems.

After having gained confidence on the computational aspects of the approach, we applied the method to study DM coupled spins in nano-disk systems. It happens that the magnetic dipole-dipole (DD) and the chiral DM interactions between nearest neighboring spins are comparable in magnitude in transition metal oxides. In particular, the effects of the DD interaction on the physical properties of magnetic nanosystems cannot be simply neglected due to its long-range character. For these reasons, we investigated the interplay of these two interactions and studied their combined effects upon the magnetic vortical structures of monolayer nanodisks [5]. We found out from our computational results that, in the presence of Heisenberg exchange interaction, a sufficiently strong DD interaction is able to induce a single magnetic vortex on a small nanodisk. A strong DM interaction usually gives rise to a multi-domain structure which evolves as a function of the temperature. In this circumstance, if a weak DD interaction is further considered, the multi-domains merge to form a single vortex in the whole magnetic phase. It was noted that, if only the Heisenberg exchange and chiral DM interactions are considered in simulations, the transition temperature is simply proportional to the size of the total spin (squared).

C) <u>Properties of a finite one-dimensional electron gas (1DEG) or two-dimensional electron gas (2DEG) model under various geometries:</u>

We studied the properties of small quantum Hall systems of electrons in a finite square geometry for a standard Coulomb interaction potential between particles. We adopted the Landau gauge which is the suitable one for a square geometry. We calculated all quantities of interest that correspond to systems with an arbitrary number of particles. In order to involve undergraduate students in meaningful research, we also "simplified" the problem to a semi-classical model that the undergraduate students would understand better. The basic idea was to treat the electrons not as point-like particles, but as extended 1D "rod-like/stripe" objects [1] with their charge uniformly spread (this treatment is plausible for the case of electrons moving in 2D in presence of a perpendicular magnetic field when the Landau gauge is used). In such a case, we obtained the precise form of the effective/modified interaction potential between the resulting "rod-like/stripe" structures in an elongated quasi-1D system [22]. This model is also important to mathematical physics studies as well as biological systems that routinely deal with elongated "rod-like/stripe" structures.

We calculated various properties of a finite one-dimensional electron gas (1DEG) model for any given arbitrary number of particles [21]. The homogeneous electron gas model has been quite successful to predict the bulk properties of systems of electrons at various densities. In many occasions, a simplified free homogeneous electron gas model represents a powerful first approximation to a real system. Despite our considerable knowledge on the bulk properties of a homogeneous electron gas, advances in nanoscience and nanotechnology call for a greater effort to understand the opposite limit of small finite systems of electrons with size-dependent properties. We provided a detailed description of the properties of a finite fully spin-polarized (spinless) free homogeneous 1DEG. We derived exact analytical results for various quantities such as the one-particle density function, two-particle density function, one-particle density matrix, pair correlation function and energy of finite systems with an arbitrary number of electrons.

We calculated the energy and various properties of a finite two-dimensional electron gas (2DEG) model [20]. We found some very interesting non-monotonic variations of the energy of the system when the finite number of electrons changes value. We adopted a Hartree-Fock approach and calculated the energy of a finite 2DEG system confined to a region that is treated as a positive jellium background. The electrons are considered fully spin-polarized (spinless) and interact with a Coulomb potential. The calculation of the exact potential energy of electrons in a finite square jellium domain is very challenging since the mathematical expressions depend in each component of particle's position and not the radial distance from the center of the domain. In order to address this issue we introduced an approximation to the problem. We assessed the quality of this approximation and discussed instances where its use is not only desirable, but also fairly accurate. The results give a correct picture of how the energy of the finite system evolves towards the bulk value as the size of the system increases.

D) <u>Anisotropic behavior in low-dimensional systems and/or anisotropic quantum Hall-like phases of electrons</u>:

We investigated anisotropic behavior in low-dimensional systems and/or anisotropic quantum Hall-like phases of electrons from the perspective of liquid crystalline phases. In our view, the source of anisotropy in certain quantum Hall systems (with GaAs as a host) is the piezo-electric effect that comes from the host substrate [7]. The piezo-electric effect effectively leads to an anisotropic interaction between electrons (a similar effect is also attributed to an effective anisotropic mass). An anisotropic interaction potential may strongly influence the stability of various quantum phases that are close in energy since the overall stability of an electronic system is very sensitive to local order. As a result, there is possibility that various anisotropic electronic phases may emerge even in the lowest Landau level in regimes where one would not expect them. We studied the state with filling factor 1/6 in the lowest Landau level. This state is very close to the critical filling factor where the liquid-solid transition takes place. We investigated whether an anisotropic Coulomb interaction potential is able to stabilize an anisotropic electronic liquid state at this filling factor. We described such an anisotropic state by means of a liquid crystalline wave function with broken rotational symmetry which can be adiabatically connected to the actual wave function for the corresponding isotropic phase. We performed quantum Monte Carlo simulations in a disk geometry [3] to study the properties of the anisotropic electronic liquid state under consideration. The findings [8] indicate stability of liquid crystalline order in presence of an anisotropic Coulomb interaction potential. The results are consistent with the existence of an anisotropic electronic liquid state in the lowest Landau level.

We take the opportunity to remark that certain aspects of this research were also well suited to the level of preparation of undergraduate students. Undergraduate students were actively engaged in all phases of the project. In particular, they worked on a study that dealt with the concept of anisotropic mass. Their efforts ultimately led to a publication of a peer-reviewed paper [6]. The focus was on the cyclotron motion of a charged particle subject to a uniform magnetic field which is thoroughly described in many classical physics textbooks. Although the assumption of a particle with isotropic mass is taken for granted in classical physics, a key concept in condensed matter physics is that of particles that have an effective anisotropic mass such as electrons in the context of band structure studies of solids. Since some exposure to the concept of anisotropic mass is important within the framework of classical physics, we considered the cyclotron motion of a charged particle with anisotropic mass in the presence of a uniform magnetic field. The exact solution of this problem exposes a broad audience of readers to concepts in condensed matter physics that are rarely mentioned within the framework of classical physics. Key ideas on the topic were illustrated in a pedagogical way by considering specific examples that show how an anisotropic mass modifies the cyclotron motion of a charged particle.

We completed a detailed study of the properties of a specific class of anisotropic quantum Hall liquid states of electrons that lack translational invariance [15]. We used a novel class of anisotropic Fermi wave functions to this effect. We used this approach to explain recent unanticipated findings that indicate the presence of an anisotropic fractional quantum Hall state in the lowest Landau level. The key expectation of our work was that novel anisotropic liquid phases of electrons may stabilize even in a strong magnetic field regime where normally one expects to see only isotropic quantum Hall liquid states. Although the energy of the anisotropic wave function under consideration was somehow higher than the energy of the competing uniform isotropic liquid phases, we still believe that additional refinements of the approach may ultimately lead to more interesting results.

E) <u>Role of finite size, confinement and geometry on various properties of nano-systems:</u>

The research in this direction spanned several topics such as**: (i)** Confined two-dimensional electronic systems under various geometries**; (ii)** Confined spin-polarized fermion systems in the quantum regime; and **(iii)** Models of nano-structures and/or finite systems with various geometries and shapes.

(i) We studied the minimum energy equilibrium configurations of a classical two-dimensional system of point charges confined by a triangular, square and disk region with a hard-wall boundary [10]. It is assumed that the point charges interact via a repulsive Coulomb interaction potential. Monte Carlo simulations with the annealing algorithm suggest that the equilibrium configurations of a given system are strongly influenced by the external (isotropic/anisotropic) geometry of the hard-wall boundary. The numerically obtained energies extrapolated in the bulk limit converge to the expected continuum equilibrium values (when known). It is found that the equilibrium charge distribution is non-uniform in the continuum limit for all the hard-wall confining regions considered. Since the continuum equilibrium charge distribution is not known for the case of an equilateral triangle or a square domain we choose to compare the numerically obtained bulk energy results to corresponding values for a uniformly charged system [9, 17]. We calculated exactly the electrostatic energy of various uniformly charged planar objects and used the findings to assess the discrepancy between such results and the numerically obtained equilibrium bulk energy values for the cases of an equilateral triangle and a square hard-wall boundary. These estimates help us understand how an anisotropic boundary with the shape of an equilateral triangle or square influences the energy of an equilibrium charge distribution. The results indicate that the energy discrepancy between equilibrium and uniform charge distributions in the continuum limit is not very large. It is found that the order of magnitude of the relative deviation of the energy for all three different planar domains considered here is approximately the same.

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Calculation of spin properties is difficult even for simple models [13]. In order to understand the impact that geometry/shape has on the properties of a finite 2DEG system, the PI together with undergraduate students calculated the shape-dependent energy for a 2D elliptical jellium system [18]. This result will be very useful to calculate the energy of a distorted 2DEG with elliptical Fermi surface, a system that is believed to exist under certain conditions.

(6) Bibliography

The best measurable outcome of research productivity is the number of peer-reviewed papers published by the PI and his collaborators. Below is a complete list of peer-reviewed papers published with support from this grant during the last 3-4 years.

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(7) Appendixes

N/A