National Institute of Physics

College of Science, University of the Philippines

Diliman, Quezon City 1101

Structure and Dynamics Research Program Annual Report

Period Covered: January – December 2013

Program Coordinator: Dr. Cristine Villagonzalo (1 January – 31 May 2013)

Dr. Francis Paraan (1 June – 31 December 2013)

Contents:

A. Milestones and Summary of Activities

A.1 Summary

A.1.1 Current members

Faculty Members	1) Dr. Ronald Banzon	Vice-Chancellor for Academic Affairs
	2) Dr. Cristine Villagonzalo	OEC Director
	3) Dr. Francis Paraan	
Ph.D. Students	1) Carlos Baldo III	Graduate Assistant (May - 21 July 2013)
		University Research Associate 1 (22 July - 31 December 2013)
	2) Micielle Capili	University Research Associate 1 (14 June 2012 - 30 June 2013)
	3) Neris Ilano	DOST-ASTHRDP
M.S. Students	1) Gina Tongco-Rosario	Hewlett-Packard
	2) Rona Barbarona	Instructor, UPLB
	3) Francis Bayocboc, Jr.	DOST- ASTHRDP
	4) April Cortez	PFSweb
	5) Hilton Lazo	Shifted to UP College of Law beginning Sem 1 AY 2013-2014
Undergraduates	1) Joachim Suico	Project staff
	2) Xavier Puspus	Student Assistant
	3) King Karl Seroje	Project staff
	4) Joshua Dizon	Project aide
	5) Robert Tacbad	
Apprentices	1) Rafael dela Rosa	
	2) Salvador Laurente, Jr.	
	3) John Kevin Sanchez	
	4) Ryan Carlo Tabernilla	

A.1.2 Activities / Highlights

During the summer session of AY 2012-2013, Dr. Cristine Villagonzalo mentored a college intern Gene Moses Itable, who was then a senior BS Physics student of the Polytechnic University of the Philippines. During this internship, G. Itable was learned to perform Monte Carlo simulations to study the effects of geometric frustration in Ising spin models.

Also, the Structure and Dynamics Group accepted three high school students (Ronnel Austria, Gerlito Chagas, John Caleb Roxas) from various Philippine Science High School campuses for the Summer Science Internship Program (17 April - 16 May 2013). The student interns were taught and exposed to the fundamentals of computational physics, error analysis, and numerical integration. They also attended the candidacy and colloquium presentation of SanD PhD students to expose them to the nature and conduct of scientific presentations.

Two of SanD's PhD students have advanced to candidacy in the summer session 2013. N. Ilano delivered the talk "*Implementation of quantum gates in an Ising nuclear spin chain computer with first- and second-nearest neighbor interaction*" during her candidacy examination on 3 May 2013. Her Ph. D. colloquium "*Quantum Mix: Spinning and flipping at the right tune*" followed on 16 May 2013. Further, C. Baldo completed his candidacy examination on 15 April 2013 with presentation "*Rashba and Dresselhaus Spin-Orbit Interactions in a Curved Quantum Wire*." He delivered his Ph. D. colloquium "*Spin switch via Spin-Orbit Interactions: The Gateway to Spintronics Revolution*" on 15 May 2013.

The OVPAA Balik-PhD project "Quantum entanglement in low-dimensional systems: quantum spin chains and continuum systems" (project leader: F. Paraan) formally commenced 1 June 2013. Project funds were used to procure computing infrastructure and support student researchers. The computers obtained from this grant are now being setup as a small high performance computing (HPC) cluster.

From 13-25 October 2013, an undergraduate SanD member (J. Dizon) attended the "Workshop on High Performance Computing (HPC) Architecture and Applications in the ICTP." This workshop was organized by the International Centre for Theoretical Physics (ICTP) and took place in Trieste, Italy. On the recommendation of F. Paraan, J. Dizon was able to secure partial support for international travel and full support for local accommodation. As part of this workshop Dizon gave a presentation that described the computational equipment acquired through this grant as a possible platform for high performance computing [C.3.2].

From 23–25 October 2013, three (3) SanD faculty and seven (7) SanD students participated in the 31st Samahang Pisika ng Pilipinas (SPP) National Physics Congress held at the University of San Carlos, Cebu City. In total, seven oral presentations were given and two posters were presented by SanD members. All SanD students (3

graduate students and 4 undergraduates) were able to secure financial grants to cover their conference expenses.

On 7 November 2013, SanD organized a Wolfram technical seminar. Mr. Farid Pasha, a representative of Wolfram Research, Inc. (developer of Mathematica technical computing software) was invited to present a technical seminar at the National Institute of Physics. In this technical seminar live computation demonstrations were used to highlight the use of Mathematica in education and research. This seminar was attended by a students and scientists from diverse research backgrounds. Among the 44 attendees were representatives from DOST-ASTI, UPD NIP (physics), UPD NIGS (geology), UPD IC (chemistry), UPD CoE/DCS-ICE-EEEI, UPD SE, UP PGH, UPLB, UST, and AdMU faculty.

From 10-16 November 2013, F. Paraan attended the "Conference on Frontiers of Condensed Matter Physics" at the ICTP in Trieste, Italy. Funding for international travel and accommodation was fully covered by the ICTP. The conference was composed of approximately 35 talks and a poster session on a broad range of topics in condensed matter physics. Attendance in this conference allowed the project leader to reconnect with colleagues at the ICTP and to form more connections with scientists in other countries.

From 10 December 2013 to 17 January 2014, SanD is hosting Ms. Maria Michiko Alcanzare, who is visiting from Aalto University, Finland. She is currently using the computer facilities of SanD for simulations for her research relating to numerical fluid dynamics. She is also mentoring X. Puspus in the use of open-source large scale particle simulation software to model classical fluids.

The computer cluster being built through SanD's OVPAA Balik-PhD grant is capable of being used as a small-scale HPC platform. A critical element in this transformation is the expertise of an HPC systems administrator. J. Dizon was sent to the ICTP precisely to be trained as an HPC systems administrator to achieve this goal of bringing HPC capabilities to the SanD research group. The required system configuration and HPC training started shortly after Dizon's return. The computational facility is currently in its testing and benchmarking phase, but it is already producing research results for J. Suico's upcoming B.S. thesis (March 2013) and M. Alcanzare's PhD studies.

Additionally, F. Paraan has also been communicating with Dr. Gemma Narisma (Manila Observatory), to explore the possibility of sharing SanD's computational facility with Dr. Narisma's advisees who are performing numerical work on climate models.

A.2 List of students who graduated in 2013

No SanD students graduated in 2013.

B. Research Projects

B.1 OVPAA Balik-PhD Grant

B.1.1

Project leader: Dr. Francis Paraan

Title: Quantum entanglement in low-dimensional systems: quantum spin chains and continuum systems (OVPAA-BPhD-2012-05)

Duration: 01 April 2013 – 31 May 2015

Amount: Php 1,914,000.00

Project RA: Rona Barbarona

Project staff & aides: Joachim Suico, King Karl Seroje, Joshua Dizon, Glenn Aguarte

Summary:

This project aims to establish a research subgroup within SanD that will focus on basic research on the study of quantum correlations in low-dimensional quantum models. This research is primarily theoretical in nature and the physical models of interest are known to be exactly solvable or approximately solvable. The class of physical systems to be investigated in this project include interacting quantum gases and spin systems in one and two dimensions [C.2.6-7]. These analytic results are to be complemented by numerical computations that will be performed on SanD's recently acquired computational facility and software.

Aims and objectives:

- regularly produce internationally recognized scientific papers,
- produce skilled, knowledgeable, and socially responsible undergraduates and graduates who are prepared for careers in the academe and industry,
- develop teaching materials and modules appropriate for advanced undergraduate and graduate students of physics,
- develop local expertise in the field of quantum information theory and search for means to connect physical quantities in this field with analogous quantities in statistical mechanics,
- develop competence and facility with parallel programming techniques that can improve computational times by an order of magnitude or more, and
- establish a numerical analysis facility that can serve the small-scale computational needs of other research laboratories within the National Institute of Physics and the College of Science.

B.2 NIP Faculty Grants

B.2.1

Project Leader: Dr. Ronald Banzon

Title: The effect of the Hadamard gate decomposition in the simulation of Grover's algorithm

Duration: January – December 2013

Amount: Php 42,000.00

Student involved: Neris Ilano

Other SanD member: Dr. Cristine Villagonzalo

Abstract:

"Simulation of Grover's algorithm in an Ising nuclear spin chain computer with first- and second-nearest neighbor interaction is considered. The most frequently used quantum gate in the algorithm is the Hadamard gate. We investigate the effect of its decomposition into several rotation matrices and numerically calculate the fidelity and probability of success of finding the target state. Using an appropriate decomposition, we obtain a high fidelity for different numbers of iterations. The probability of finding the target state also increased and is much closer to the ideal result." [C.2.1]

B.2.2

Project Leader: Dr. Cristine Villagonzalo

Title: Spin switching on a quantum wire with spin orbit coupling in a uniform magnetic field

Duration: January – December 2013

Amount: Php 42,000.00

Student involved: Carlos Baldo III

Abstract:

"The interplay of a uniform perpendicular magnetic field and the radius of curvature on the spin transport along a curved quantum wire with Rashba and Dresselhaus spin-orbit interactions is investigated. From the analytic calculations of the system's eigenenergies and eigenfunctions, transmission coefficients were numerically determined using transfer-matrix approach and were used to calculate the probability current densities and output polarization. Our results show that the spin orientation of the initially spin-polarized electron can be switched for smaller values of radius of

curvature of the curved quantum wire. However, the range of spin switching is largely dependent on the threading magnetic field and on the strength of the spin-orbit interactions." [C.2.3]

B.2.3

Project Leader: Dr. Francis Paraan

Project Title: Development of High Performance Parallel Computing for Structure and Dynamics Applications

Duration: January – December 2013

Amount: Php 36,000.00

Student involved: Robert Tacbad

Paper Title: Parallel Speed-up and Efficiency in Single Loop Sums and Matrix Multiplication

Abstract:

"This study aims to evaluate the performance of parallel implementations of single loop sums and matrix multiplication using the Message Passing Interface. Benchmark results were obtained from the available computing resources of the Structure and Dynamics Group (SanD). These implementations were run using 1 to 24 processors and their speed-up and effciency were calculated. Nearly ideal speed up and efficiency was observed when tasks were distributed over physical cores of a single CPU." [C.2.8]

B.3 Unfunded Research Projects

B.3.1 Percolation

Project Leaders: Dr. Ronald Banzon and Dr. Cristine Villagonzalo

Duration: January – December 2013

Students involved: Micielle Capili and Joachim Suico

Abstracts:

"The critical exponent β related to the percolation probability describes the dimensionality of a specific lattice topology. The accurate determination of β will aid in distinguishing different universality classes. This work describes the fine tuning of the Sigma method developed previously by the authors in obtaining β. The approach uses the log-log plot of the percolation probability versus the difference of the occupation probability and the percolation threshold. Considering a symmetric distribution of

points about the midpoint of this plot yields the β with (1) the lowest standard deviation and (2) the appropriate asymptotic behavior for both one and two-dimensional lattices." [C.2.2]

" A study of interest in site percolation is to determine the characteristics of other clusters formed that do not span a given space. In this work we simulate on a square lattice of size L x L and show the behavior of the mean cluster size and its associated parameters near the percolation threshold. We find that at the percolation threshold the mean cluster size is proportional to $L^{1.656}$. " [C.2.4]

B.3.2 Quantum gases

Project Leaders: Dr. Francis Paraan

Duration: January – October 2013

Collaborators: Jayson Cosme and Dr. Jose Perico Esguerra

Abstract:

"We investigate the Thomas-Fermi approach on the single particle density of a strongly interacting one dimensional bose gas under harmonic confinement with multiple localized δ barriers. We compare the resulting approximate of the density profile to exact density profiles that can be calculated for finite number of bosons. From the ground state energy, the corresponding chemical potential at $T = 0$ is used to find the radius or extent of the density cloud." [C.2.5]

C. Publications and invited talks

C.1 ISI Publications

C.1.1 R. Gammag and C. Villagonzalo. "Two-dimensional electron gas tilt-induced Landau level crossings." *Solid State Commun.* **156** (2013) 16-20.

C.2 National Conference Proceedings

The following papers are authored or co-authored by SanD members. They appear in the refereed Proceedings of the 31st Samahang Pisika ng Pilipinas (SPP) National Physics Congress held at the University of San Carlos, Cebu City, from 23–25 October 2013:

C.2.1 N. Ilano, C. Villagonzalo, and R. Banzon. "The effect of the Hadamard gate decomposition in the simulation of Grover's algorithm."
(Manuscript SPP2013- 5B-2 Oral)

C.2.2 M. Capili, R. Banzon, and C. Villagonzalo. "Determination of the percolation critical exponent as measure of dimension."
(Manuscript SPP2013-4C-6 Oral)

C.2.3 C. Baldo and C. Villagonzalo. "Spin switching on a quantum wire with spin orbit coupling in a uniform magnetic field."
(Manuscript SPP2013-5B-4 Oral)

C.2.4 J. Suico, R. Banzon, and C. Villagonzalo. "Characteristics of non-spanning clusters in a percolating two-dimensional square lattice."
(Manuscript SPP2013- PB-10 Poster)

C.2.5 J. Cosme, F. N. C. Paraan, and J. P. Esguerra. "Thomas-Fermi approach on the particle density of a Tonks-Girardeau gas in harmonic confinement with multiple delta-perturbations."
(Manuscript SPP2013- 3B-2 Oral)

C.2.6 X. Puspus and F. N. C. Paraan. "Entanglement entropy of impenetrable bosons in 1D: Effects of block length and boundaries."
(Manuscript SPP2013- 3B-7 Oral)

C.2.7 K. K. Seroje and F. N. C. Paraan. "Entanglement spectrum and entropy of two-mode squeezed vacuum states."
(Manuscript SPP-2013-3B-6 Oral)

C.2.8 R. Tacbad and F. N. C. Paraan. "Parallel speed-up and efficiency in single loop sums and matrix multiplication."
(Manuscript SPP2013-PB-09 Poster)

C.3 Invited Talks and Presentations

C.3.1 F. N. C. Paraan. "Entanglement, statistical mechanics, and parallel computing." Plenary talk given at the *31st Samahang Pisika ng Pilipinas Physics Congress*, University of San Carlos, Cebu City (October 2013).
(Plenary talk SPP2013-PS-04)

C.3.2 J. Dizon. "HPC at the Structure and Dynamics Group." Informal presentation delivered at the *Workshop on High Performance Computing (HPC) Architecture and Applications in the ICTP*, Trieste, Italy (October 2013).

D. Future Plans

D.1 Two-dimensional Electron Gas

C. Villagonzalo is continuing her research on the thermodynamic properties of two-dimensional electron gases (2DEG) at low temperatures with her MS student G. Tongco-Rosario and in collaboration with Dr. Rayda Gammag, a postdoctoral fellow at the Asia Pacific Center for Theoretical Physics, Pohang, Korea. Specifically, they are calculating the effects of an in-plane (tilted) magnetic field on the specific heat capacity

and the conductance of the 2DEG. This research is relevant to the fundamental understanding of the quantum Hall effect.

D.2 Quantum Entanglement

F. Paraan is undertaking basic research in entanglement in interacting quantum systems. Two MS students (F. Bayocboc and R. Barbarona) and two BS students (X. Puspus and K. Seroje) are performing analytic studies that are expected to produce publications in 2014 or in early 2015. F. Bayocboc is studying the work spectrum of quenched anisotropic XY Heisenberg models, R. Barbarona is exploring the dependence of entanglement on microscopic coupling constants, X. Puspus is deriving Schmidt decompositions of Bethe wavefunctions, and K. Seroje is studying entanglement in squeezed states. This research will be the basis of the respective student's thesis work, which will be defended in 2015.

D.3 Spin-orbit interactions on a curved quantum wire

Ph.D. student C. Baldo is doing his research on the effects of spin-orbit couplings in the transport of a spin-polarized electrons on a curved quantum wire under the mentorship of C. Villagonzalo. Their study is in congruence with the present issues in the emerging field of spintronics on how to effectively manipulate spin transport in spin-based electronic devices that do not require either ferromagnetic materials, external magnetic fields or both. They have already derived analytically the eigenfunctions and the eigenvalues of the system Hamiltonian. Numerical computations have already been carried out to solve several transport properties such as spin polarization, probability current densities and spin-dependent conductance. In 2014, C. Baldo will present his results in manuscript form for submission to an international peer-reviewed journal.

D.4 Percolation

C. Villagonzalo and R. Banzon are continuing their research on percolation in the presence of conducting and non-conducting impurities. J. Suico is numerically studying the influence of confinement space on the size distribution of the non-spanning conducting islands and the effect of this distribution on the percolation critical exponents. The results of this research will form the basis of J. Suico's BS thesis work, which is expected to be defended in March 2014.

D.5 Parallel computation

F. Paraan is overseeing the completion of a small HPC cluster that can be used for parallel computing tasks. In 2014, J. Dizon is expected to complete the remaining administrative (configuration) tasks for the cluster to be deployable to SanD students and collaborators at large. Since J. Dizon is graduating in 2015, he is also in charge of administering a crowd-sourced resource website (a 'wiki') that can be used by future cluster users. The construction of the HPC cluster and wiki will constitute J. Dizon's undergraduate thesis project, which is expected to be completed in 2015. On the

software side, R. Tacbad is learning to optimize the use of the cluster hardware by writing natively parallel code using standard open-source libraries as templates. The benchmarks and optimizations that R. Tacbad will produce in 2014 will be used to improve the performance of the numerical codes used by SanD. Also, the recent collaboration of X. Puspus and M. Alcanzare will add large-scale particle simulations (lattice Boltzmann fluids and molecular dynamics) to the list of core numerical competencies of SanD in 2014.

D.6 Quantum search algorithms in an Ising spin quantum computer

Ph. D. student N. Ilano is simulating Ising spin quantum computers under the mentorship of C. Villagonzalo and R. Banzon. Their future goal is to simulate generalized quantum search algorithms on classical simulations of an Ising spin quantum computer. They have already simulated Grover's algorithm in an Ising spin chain quantum computer, taking into account the first- and second-nearest neighbor interactions with four spins (qubits). However, they still have to address the degeneracy of the state transitions that come into play when the size of the database is increased. A more general Ising spin system can be considered to account for these unwanted degenerate transitions. One of the possible solutions that they are currently working on is to introduce an external field with an effective magnitude that depends on the coupling constants between interacting spins. The results of this research will be submitted to an international peer-reviewed journal as part of the requirements of N. Ilano's Ph. D. Physics program.

D.7 2014 Summer Internship

With the success of the 2012 and 2013 Summer Science Internship Program of the Philippine Science High School at the National Institute of Physics, SanD has committed to accepting at most four high school students as interns this summer 2014.