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 2014

Program Coordinator: Dr. Francis Paraan

Abstract: In 2014, the Structure and Dynamics (SanD) Research Program increased in size and output compared to recent years and continues to grow. Total membership jumped 25% (from 20 to 25 members). Two students graduated (1 MS and 1 BS) this year with several more officially on "graduating" status. Two papers were published in highly regarded ISI-listed journals and three research works have been presented in international conferences and schools. Five presentations (4 oral and 1 poster) were accepted in this year's Samahang Pisika ng Pilipinas Physics Conference.

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A. Milestones and Summary of Activities

A.1 Summary

A.1.1 Current members

Faculty Members	1) Dr. Ronald Banzon Associate Professor	Vice-Chancellor for Academic Affairs (up to 30 Apr 2014) On Sabbatical from 01 Aug 2014
	2) Dr. Cristine Villagonzalo Associate Professor	OEC Director (up to 31 May 2014) PD Associate (01 Jul—31 Dec 2014)
	3) Dr. Francis Paraan Assistant Professor	SanD Program Coordinator
Ph.D. Students	1) Carlos Baldo III	University Research Associate 1 (01 Jan—31 Dec 2014)
	2) Neris Ilano	DOST-ASTHRDP
M.S. Students	1) Gina Tongco-Rosario	Hewlett-Packard (Graduated: Summer 2014)
	2) Rona Barbarona	Instructor, UPLB
	3) Francis Bayocboc, Jr.	DOST- ASTHRDP
	4) April Cortez	
	5) Aura Villaruel	NIP Graduate Assistant (01 Aug—31 Dec 2014)
Undergraduates	1) Joachim Suico	Project staff (Graduated: Sem 2 AY 2013-14)
	2) Joshua Dizon	Project aide
	3) Xavier Puspus	NIP Student Assistant (04 Nov 2013—31 Mar 2014)
	4) King Karl Seroje	Project staff
	5) Robert Tacbad	Project aide
	6) Salvador Laurente, Jr.	Project aide
	7) Rafael dela Rosa	Project staff
	8) John Kevin Sanchez	Project aide
	9) Ryan Carlos Tabernilla	Project aide
Apprentices	1) Geronimo Acosta	
	2) Patrick Elegado	
	3) Nicholas Colina	
	4) Robertson Esperanza	
	5) Zed Harold Fernandez	
	6) Lean Louiel Peria	

A.1.2 Activities/Highlights

On 13 February 2014, four SanD members participated in the 6th Asian Computational Materials Design Workshop held at de la Salle University (DLSU) in Manila. Cristine Villagonzalo delivered a talk "Fundamental studies and simulation of nanostructured materials" [C.4.1]. Francis Paraan and two students (Joshua Dizon and Robert Tacbad) attended the afternoon lectures on density functional theory. During this visit, Professor Nelson Arboleda of DLSU gave a short tour of the high performance computing (HPC) cluster of DLSU, which is similar to the heterogeneous cluster being built in SanD. Discussions between Prof. Arboleda and Francis Paraan opened up channels for scientific exchange with DLSU researchers on the simulation of materials using density functional theory (DFT) and molecular dynamics.

From 27 February to 28 February 2015, PhD candidate Neris Ilano delivered a contributed talk at the 3rd National DOST-SEI ASTHRDP-NSC Scholars' Conference in Manila [C.4.2]. Neris's graduate studies are funded by DOST-ASTHRDP.

At the end of the second semester of AY 2013-2014 (March 2014), Joachim Suico successfully defended his BS thesis "Characteristics of Non-Spanning Spatial Structures and its Effects on Criticality and Percolation in a Two-Dimensional Square Lattice with Constrained Sites," with co-advisers Ronald Banzon and Cristine Villagonzalo. His graduation from the BS Physics program was approved soon after. Joachim is SanD's 26th BS degree graduate and is currently working for an internet security company.

In the summer session of AY 2013-2014 (April-May 2014), two UP Manila BS Applied Physics students, Shannen Andrade and Krishna Godino, joined SanD as summer interns under NIP's on-the-job training (OJT) program. Both students were hired as project staff of the OVPAA Project BPhD 2012-05 [B.1.1]. In the first weeks of their internship, they made an information video (youtu.be/8QYE4UxRWdc) that highlights the relationship between the scientists and alumni of SanD and the International Centre for Theoretical Physics (ICTP). The video also emphasizes the variety of career paths taken by SanD graduates as an information campaign to encourage students to pursue a science degree. Shannen and Krishna also trained in the use of computational software for image processing tasks. Due to their background as health physics students, they worked on developing an application that allows users to identify and count cells or bacterial colonies in digital micrographs.

SanD also participated in the 2014 Summer Science Internship Program (SSIP) of the Philippine Science High School (PSHS) System and NIP (21 April-16 May 2014). Four PSHS students, Meg Dizon, Julia Jumalon, Maikee Tamara Lagasca, and Cleo Clarice Vibas, were mentored in this program. They used SanD's computational facilities to develop visualizations of root-finding and numerical integration techniques.

At the end of the summer session May 2014, Gina Tongco-Rosario successfully defended her MS thesis "Specific Heat and Magnetization of Two Dimensional Electron Gas (2DEG) with Spin Interactions in Tilted Magnetic Field," with co-advisers Cristine Villagonzalo and Rayda Gammag (postdoctoral fellow at the APCTP). After the approval of her graduation from the MS Physics program, she became the 15th MS graduate of SanD. Gina continues working for Hewlett-Packard.

Also in May 2014, SanD launched its new website at www.nip.upd.edu.ph/sand. It contains all publications and conference presentations of SanD members and allows faculty to post their teaching materials. The SanD website also highlights the extension work of SanD members, such as the SSIP and OJT programs. This website runs on an industry-standard content management system (Drupal) that is also used for the main NIP website.

From 01 August 2014, Ronald Banzon is officially on a one year sabbatical. While on sabbatical, he continues to advise and mentor his PhD student Neris Ilano.

From 20 August to 24 August 2014, SanD graduate students Rona Barbarona and Francis Bayocboc, Jr. attended the 14th Asian Quantum Information Science Conference held in Kyoto, Japan. They presented two research posters to an international audience and attended talks delivered by experts in quantum information science. Rona's participation [C.2.1] was fully supported by OVPAA Project BPhD 2012-05 [B.1.1], while Francis's participation [C.2.2] was co-funded by OVPAA Project BPhD 2012-05 and a DOST-ASTHRDP grant. This exposure to international scientific exchanges is a good learning experience for them, especially since they are following an academic career path.

From 16 September to 25 September 2014, SanD PhD candidate Neris Ilano attended a summer school at the Okinawa Institute of Science and Technology (OIST). The theme of this school was Coherent Quantum Dynamics (CQD2014) scientists and graduate students from several countries attended it. She presented a research poster [C.2.3] during the School's poster session and attended several lectures by prominent scientists working on coherent quantum systems. Neris's attendance in CQD 2014 was supported by the OIST Graduate University and the DOST-ASTHRDP.

From 17 October to 20 October 2014, SanD members attended the 32nd Samahang Pisika ng Pilipinas Physics Congress held in UP Diliman. Three faculty members, one URA (Carlos Baldo III), one PhD student (Neris Ilano), and four undergraduates (Rafael de la Rosa, Robert Tacbad, John Kevin Sanchez, and Ryan Carlos Tabernilla) registered for the conference. Funding was secured from NIP, UP Diliman, and also partially from OVPAA Project BPhD 2012-05. A total of four oral talks and one poster were presented by SanD [C.3].

On 01 December to 02 December 2014, SanD members registered and participated in the 2014 UP OVPAA Research Symposium held at the NIP. Francis Paraan delivered a talk on his Balik-PhD research project, which gave an overview of the accomplishments made in the first 18 months of the project [C.4.3].

A.2 List of students who graduated in 2014

A.2.1. MS Physics: Gina Rose Tongco-Rosario (Summer 2014)

MS Thesis: *Specific heat and magnetization of a two-dimensional electron gas with spin-interactions in tilted magnetic fields*

Adviser: C. Villagonzalo. Co-adviser: R. Gammag

A.2.2. BS Physics: Joachim Suico (2nd Sem AY 2013-2014)

BS Thesis: *Characteristics of non-spanning spatial structures and its effects to criticality and percolation in a two-dimensional square lattice with constrained sites*

Co-advisers: C. Villagonzalo and R. Banzon

B. Research Projects

B.1 UP System

B.1.1 OVPAA Balik-PhD Grant

Project leader: 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, Rafael dela Rosa, King Karl Seroje, John Kevin Sanchez, Ryan Carlos Tabernilla, Salvador Laurente, Jr., Joshua Dizon, Robert Tacbad

Other students: Xavier Puspus

Summary:

This project is a fundamental study on the nature of quantum correlations in the form of entanglement in low-dimensional systems. This research is primarily theoretical and computational in nature and the physical models of interest are known to be exactly solvable or approximately solvable. Emphasis so far is on entanglement between modes (or species), which is only recently gaining more attention in the quantum information community. Funds from this project are also used to procure computational hardware needed to set up a heterogeneous computation cluster that

involves several CPU cores and GPU cores networked together. This infrastructure allows SanD members to parallelize computational tasks that are needed for their research.

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 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 in the form of a heterogeneous computing cluster.

Paper Title: Entanglement spectrum and number fluctuations in the spin-partitioned BCS ground state.

Abstract: "We study entanglement between the spin components of the BCS ground state by calculating the full entanglement spectrum and the corresponding von Neumann entanglement entropy. The entanglement spectrum is effectively modeled by a generalized Gibbs ensemble (GGE) of noninteracting electrons, which may be approximated by a canonical ensemble at the BCS critical temperature. We further demonstrate that the entanglement entropy is jointly proportional to the pairing energy and to the number of electrons about the Fermi surface (an area law). Furthermore, the entanglement entropy is also proportional to the number fluctuations of either spin component in the BCS state." [C.1.2]

Paper Title: Mode entanglement in squeezed coherent and displaced squeezed states.

Abstract: "We study mode entanglement in four quantum states (coherent state, squeezed vacuum state, displaced squeezed state, squeezed coherent state), which are generated from a bosonic two-mode vacuum state by the action of displacement and squeezing operators. The mode entanglement entropy in these states is calculated and shown to depend only on the squeezing magnitude." [C.3.3]

B.2 UP Diliman Grants

B.2.1 OVCRD PhD Incentive Award

Project leader: Francis Paraan

Title: Quenches in solvable spin-chain models (Project No. 141420)

Duration: 01 October 2014 – 30 September 2015

Amount: Php 300,000.00

Project RA: Hiring to commence January 2015

Project staff & aides: Hiring to commence January 2015

Summary:

The proposed research is a theoretical investigation of the consequences of non-adiabatic changes (quantum quenches) in the Hamiltonian of the Heisenberg XY model. This work extends the results of previous workers who have studied such quenches in the quantum Ising model, which is a special case of the more general XY model. These interaction quenches are important in the description of non-adiabatic processes, such as those employed in certain quantum computing applications. The proposed research budget will be used primarily for expanding the current computing infrastructure of the proponent, acquire graduate and research level textbooks that are not available locally, and provide honoraria for his advisees, and support conference travel for graduate students working on the project.

Aims and objectives:

The general goal of this project is to study the work statistics and dynamics of a transverse XY spin-1/2 chain which is driven non-adiabatically across different quantum critical boundaries via quenching of its anisotropy parameter and the transverse magnetic field.

The specific objectives of this project are:

- calculate the amplitude of the Loschmidt echo of the spin-1/2 XY model right after a sudden quench of the anisotropy parameter and the transverse magnetic field at zero temperature,
- calculate the characteristic function and the probability density function of the work done on the system by the quantum quench,
- compute the entropy associated with the quenching of the system,
- analyze the quenched XY model at finite temperatures.

B.3 NIP Faculty Grants

B.3.1

Project Leader: Dr. Ronald Banzon

Title: Numerical Precision and Number of Grover Steps in an Ising Nuclear Spin Computer.

Duration: January – December 2014

Amount: Php 42,000.00

Student involved: Neris Ilano

Paper Title: Working precision in a simulation of Grover's algorithm in an Ising spin system.

Abstract: "We consider the simulation of Grover's algorithm in an Ising nuclear spin chain computer with first- and second-nearest neighbor interaction. The algorithm is simulated using different working precision. We calculate the fidelity as a function of $\pi/2$- and π-pulses and investigate the precision of the success probability of the target state. The fidelity is constrained by the set working precision of the computer system. A reduction of precision is also observed as you increase the number of iterations that restricts the size of the database to effectively simulate the algorithm. The amount of decrease is dependent on the decomposition of pulses." [C.3.2]

B.3.2

Project Leader: Dr. Cristine Villagonzalo

Title: Magnetoconductance studies in a curved quantum wire with spin-orbit coupling effects

Duration: January – December 2014

Amount: Php 42,000.00

Student involved: Carlos Baldo III

Paper Title: Magnetoconductance of a spin-polarized electron along a curved one-dimensional wire

Abstract: "In this work, we revisit our transport studies on the motion of a spin-polarized electron along a curved quantum wire under the presence of a uniform perpendicular magnetic field **B** and the Rashba and Dresselhaus spin-orbit couplings. Then from the

derived output transmission coefficients, we numerically determine the magnetoconductance of the electron motion along the curved wire. Our results agree from our earlier reports that for large effective spin-orbit coupling, the effects of **B** on spin switching is reduced. Moreover, we found that for a given energy, the desired high magnetoconductance ratio can be achieved by tuning **B**. Finally, due to adiabatic transport, the magnetoconductance decreases if one increases the radius of curvature, *R*, of the wire." [C.3.1]

B.3.3

Project Leader: Dr. Francis Paraan

Project Title: High Performance Parallel Implementation of Molecular Dynamics and Monte Carlo Computations.

Duration: January – December 2014

Amount: Php 36,000.00

Student involved: Robert Tacbad, Joshua Dizon, Ryan Carlos Tabernilla, John Kevin Sanchez

Paper Title: Lateral Motion of a Suspended Spherical Particle between Two Parallel Moving Walls

Abstract: "This study aims to observe the behavior of a spherical particle when it is suspended in a fluid which is contained between two parallel walls. A simulation was done using the molecular dynamics LAMMPS. It was observed that the particle tends to move towards the wall nearer to it and acquires a greater displacement when it is placed closer to a wall." [C.3.4]

Paper Title: Speed-up and Efficiency of Parallelized Monte Carlo Integration on Homogeneous and Heterogeneous Clusters

Abstract: "We evaluate the performance of parallelized Monte Carlo integration algorithms on homogeneous and heterogeneous clusters of the Structure and Dynamics Laboratory. In this study, intrinsic pseudorandom number generators for Fortran and Python were used and parallelization achieved by MPI libraries. On an example using 10^9 samples, the parallelized Python code proved to be scalable on a cluster of up to 44 processors. The Fortran parallelized code performed less well on scalability but had a much shorter execution time. It was also observed that the overhead cost of parallelization saturates as the number of

processors used increased." [C.3.5]

C. Publications and invited talks

C.1 ISI Publications

C.1.1 C. Baldo III and C. Villagonzalo. "Spin-orbit coupled transport in a curved quantum wire." *Physica E.* **63** 93-98 (2014). DOI: 10.1016/j.physe.2014.05.013 (IF: 1.856)

C.1.2 X. M. Puspus, K. H. Villegas, and F. N. C. Paraan. "Entanglement spectrum and number fluctuations in the spin-partitioned BCS ground state." *Phys. Rev. B* **90**, 155123 (2014). DOI: 10.1103/PhysRevB.90.155123 (IF: 3.664)

C.2 International Conference/School Presentations

C.2.1 R. F. Barbarona, F. N. C. Paraan. "Integer effects in the spin-orbit entanglement entropy in a 2D electron system with Rashba interactions." Poster presented at the 14th Asian Quantum Information Science Conference, Kyoto (20-24 August 2014).

C.2.2 F. A. Bayocboc, Jr., F. N. C. Paraan. "Work fluctuations in quantum quenches in the XY model." Poster presented at the 14th Asian Quantum Information Science Conference, Kyoto (20-24 August 2014).

C.2.3 N. Ilano, C. Villagonzalo, and R. Banzon. "Simulation of Grover's algorithm with spatially-dependent coupling constant." Poster presented at the 2014 Okinawa School in Physics: Coherent Quantum Dynamics, Okinawa (16-25 September 2014).

C.3 National Conference Proceedings

The following papers are authored or co-authored by SanD members. They appear in the refereed Proceedings of the 32nd Samahang Pisika ng Pilipinas (SPP) National Physics Congress held at the University of the Philippines Diliman, Quezon City, from 17-20 October 2014:

C.3.1 C. F. Baldo III and C. Villagonzalo. "Magnetoconductance of a spin polarized electron along a curved one-dimensional wire." (SPP2014-1A-6 Oral)

C.3.2 N. Ilano, C. Villagonzalo, and R. Banzon. "Working precision in a simulation of Grover's algorithm in an Ising spin system." (SPP2014-5A-2 Oral)

C.3.3 R. S. dela Rosa, K. K. R. Seroje and F. N. C. Paraan. "Mode entanglement in squeezed coherent and displaced squeezed states." (SPP2014-5A-7 Oral)

C.3.4 R. C. Tacbad, J. G. A. Dizon, and F. N. C. Paraan. "Lateral motion of a suspended

spherical particle between two parallel moving walls." (SPP2014-PB-4 Poster)

C.3.5 R. C. M. Tabernilla, J. K. R. Sanchez, J. G. A. Dizon, and F. N. C. Paraan. "Speed-up and efficiency of parallelized Monte Carlo integration on homogeneous and heterogeneous clusters." (SPP2014-2C-6 Oral)

C.4 Invited Talks and Presentations

C.4.1 C. Villagonzalo. "Fundamental studies and simulation of nanostructured materials." Invited talk given at the 6th Asian Computational Materials Design (CMD) Workshop—Philippines, DLSU Manila (13-15 February 2014).

C.4.2 N. Ilano. "Position Variation of the Ancilla Qubit in Grover's Algorithm." Contributed talk at the 3rd National DOST-SEI ASTHRDP-NSC Scholars' Conference, Manila (27-28 February 2014).

C.4.3 F. N. C. Paraan. "Quantum mode entanglement and building a parallelized computing cluster." Invited talk given at 2014 UP OVPAA Research Symposium, NIP, UP Diliman (1-2 December 2014).

D. Future Plans

D.1 Spin transport and spintronics

C. Villagonzalo will continue work with PhD candidate C. Baldo on the effects of spin-orbit coupling (SOC) on spin currents and other transport properties in quantum wires. They will study spin transport in the presence of modulated "on" and "off" SOCs along segments of the wire. The results of this study will be submitted to an international peer-reviewed journal as part of the requirements of C. Baldo's Ph.D. Physics program. C. Villagonzalo will also work with graduate student A. Cortez on studies of spin injection in Ferromagnet-Semiconductor tunnel structures. They seek a theoretical models that account for the large spin accumulation and short lifetimes extracted from electrical Hanle signals. In particular, they will examine the applicability of resonance-tunneling magnetoresistance theories and its possible modifications in ferromagnet-insulator-nonmagnetic (F-I-N) junctions.

D.2 Thermal transport studies in 2DES

C. Villagonzalo, R. Gammag and G. Tongco-Rosario will continue their work to establish the nature of the specific heat capacity of a 2DES in two-dimensional electron systems (2DES) in an applied magnetic field. New graduate and undergraduate students will be recruited on board this project in 2015 and will be assigned to work on the effects of various tunable parameters such as different sources of spin-orbit interaction strength, magnetic field orientation and temperature. This work will consider possible 2DES thermoelectric transport applications such as its thermal conductivity. Since the 2DES acts as the transport layer, this study will serve as a benchmark for heat

conduction applications in confined systems such as those in the transport region of semiconductor heterostructures.

D.3 Quantum entanglement

F. Paraan is undertaking basic research in entanglement in interacting quantum systems. Recent emphasis has been on entangled modes in many-body systems and the construction of effective thermal models of entangled subsystems. MS student R. Barbarona is posed to submit an article on her work on spin-orbit entanglement in a candidate spin Hall system to an ISI-listed journal. We aim for publication prior to her expected MS Physics graduation in June 2015. Meanwhile, two undergraduates, K. Seroje and R. de la Rosa, are preparing a pedagogical article for journal submission that discusses the links between von Neumann entanglement entropy and Gibbs entropy in quantum optical and coherent matter states. K. Seroje aims to make the submission prior to graduation.

D.4 Quantum quenches

With new funding from the OVCRD [B.2.1], F. Paraan continues his research on quantum quenches in solvable spin chains. Preliminary results for arbitrary quenches in the Heisenberg XY model has already been presented in an international conference [C.2.2]. MS student F. Bayocboc, Jr. is currently applying for acceptance in another international conference in South Africa to present the rest of his results. He targets a paper submission and acceptance before graduating from the MS program in June 2015.

D.5 Parallel computation and GPU computing

In the following year, SanD expects to use its new GPU processors (total 3456 GPU cores) for computational tasks using its high-performance computing cluster (HPC). Parallelization over GPU cores requires Single Instruction Multiple Data (SIMD) implementation, which is suited for Monte Carlo methods and linear algebra tasks (identical instructions applied to independent data registers). We aim to use this additional computational power for SanD's numerical research on fluid dynamics and percolation and electronic structure simulations. The electronic structure calculations will be performed by incoming PhD student Alexandra Santos-Putungan (MSEP). With the current systems/HPC administrator Joshua Dizon expected to graduate in June 2015, training for a new systems/HPC administrator is commencing. Furthermore, channels have been opened between F. Paraan and Prof. A. Lluisma who is the Director of the Core Facility for Bioinformatics. We expect collaborations on the development of computational tools with applications to bioinformatics in the future.

D.6 Quantum algorithms

R. Banzon, C. Villagonzalo, and N. Ilano will continue the study of simulating Grover's quantum search in an Ising nuclear spin chain quantum computer. The variation of the

coupling parameter in the radio-frequency pulse applied to a Hamiltonian with spatially-dependent coupling constant will be considered. This is to obtain the fidelity profile of the algorithm as we increase the number of iterations to find a single target state. The effect of the position of the ancilla qubit to the probability of finding the target state will also be investigated. The objective of this study is to put forward a general framework of the quantum search algorithm for large number of spins.

D.7 2015 Summer Internship

With the continued success of the 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 2015.