The Winnipeg Institute for Theoretical Physics¹ Annual Report

September 2004 – August 2005

¹Web site: http://www.physics.umanitoba.ca/research/witp.html

1 Director's Narrative Report

The Winnipeg Institute for Theoretical Physics was created to support theoretical physics research in Manitoba. It has carried out this mandate by encouraging collaboration between members of the Institute and by financially supporting workshops, visiting colloquium speakers, and short and long term visits by research collaborators of international standing. The permanent members of this Institute are drawn from Brandon University, the University of Manitoba, and the University of Winnipeg.

The past year was the 14^{th} year of the Institute's existence. As usual the Institute sponsored a series research colloquia by out-of-province visitors as well as Institute members. Associated with the Permanent Members were research associates, postdoctoral fellows, and graduate students.

For the 2004–2005 academic year, the list of invited speakers is found in section 4.1. Visiting scientists whose stay lasted longer than one week are listed in section 4.2. The cumulative list of graduate degrees awarded appears in section 4.3. and the published research work of associate members/graduate students and of members are found, respectively, in sections 4.4 and 4.5. The total number of refereed publications by full members listed in section 4.5 is 43 for years 2003 and 2004. These numbers do not count twice those that are collaborative publications among members of the Institute. The research associates and postdoc members published 13 refereed papers. Section 5.1 contains a summary of income and expenditures for the period September 1, 2004 to August 31, 2005. The plans for the coming year include a program of invited speakers, visiting research collaborations, and the promotion of postgraduate and postdoctoral research.

Essentially all of the funds available to the Institute are spent for workshop and colloquium activities and for travel expenses of visiting scientists. The Institute has no technical support staff or administrative staff. All the administrative work is done on a volunteer basis by the members of the Institute. The Institute's funding is substantially supplemented by contributions from the NSERC grants of individual members in pursuing the Institute's mandate.

During the past academic year, the Institute's Executive Committee has consisted of T. A. Osborn. Past-Director (Manitoba) and R. Kobes, Director (Winnipeg).

2 Current List of Members (September, 2005)

2.1 Permanent Members

- B. Bhakar¹, Ph.D. (Delhi) [Director, Jan. June 00]
- P.G. Blunden¹, Ph.D (Queen's) [Director, 93-94]
- M.E. Carrington³, Ph.D. (SUNY, Stony Brook)
- T. Chakraborty¹, Ph.D. (Dilbrugarh University, India)
- J. D. Fiege¹, Ph.D. (McMaster)
- T.D. Fugleberg³, Ph.D. (UBC)
- R.L. Kobes², Ph.D. (Alberta) [Director, 97-98]
- G. Kunstatter², Ph.D. (Toronto) [Director, 91-92]
- P.D. Loly¹, Ph.D. (London) [Director. Fall 99]
- T.A. Osborn¹, Ph.D. (Stanford) [Director, 92-93, 02-04]
- B.W. Southern¹, Ph.D. (McMaster) [Director, 90-91]
- J.P. Svenne¹. Ph.D. (M.I.T.) [Director, 95–96]
- G.C. Tabisz¹, Ph.D. (Toronto)
- J.M. Vail¹, Ph.D. (Brandeis) [Director, 98-99]
- D.W. Vincent², Ph.D. (Toronto) [Director, 94-95]
- J.G. Williams³, Ph.D. (Birmingham) [Director, 96-97]
- M. Whitmore¹, Ph.D. (McMaster)

¹University of Manitoba

²University of Winnipeg

³Brandon University

2.2 Associate Members

Research Associates

- A. Borodich (Whitmore) July '04- present
- R. E. Cameron (Tabisz) 1995- present

Postdoctoral Fellows

- Jose Martinez-Resco (Carrington) August 2004 August 2005.
- Daria Ahrensmeier (Carrington, Kobes. Kunstatter) Feb. '02- present
- Marco Califano (Chakraborty) July '04 present
- Weixing Qu (Tabisz) 2001– present

2.3 Graduate Students

- Miraseed Zelli (M.Sc.) (Southern)
- Aleksandrs Alexsejevs (Ph.D.) (Blunden)
- Svetlana Barkanova (Ph.D.) (Blunden) GRADUATED 2004
- Jason Bland (Ph.D.) (Kunstatter)
- Edward Kavalchuk (Ph.D.) (Carrington/Kobes)
- Amra Peles (Ph.D.) (Southern) GRADUATED 2004
- A. J. Penner (M.Sc.) (Kobes) GRADUATED 2004
- Andrew Senchuk (M.Sc.) (Tabisz)
- J. Medved (Ph.D.) (Kunstatter) GRADUATED 2000
- T. Melde (Ph.D.) (Svenne) GRADUATED 2001
- Slaven Peles (Ph.D.) (Kobes) GRADUATED 2001

2.4 Undergraduate Research Students 2004-2005

- D. K. Chevrier (J.M. Vail)
- Chris Wyenberg, (Southern)
- Jason Wyenberg. (Southern)
- Todd Kruk, May August 2005 (NSERC summer undergraduate research award) [Carrington / Fugleberg].
- Kai Choy, May August 2005 (NSERC summer undergraduate research award) [Carrington / Fugleberg].
- Vince Bagnulo (Kunstatter)
- Dave Ostapchiuk (Kunstatter)
- Gina Passante (Kobes)

3 Research Interests of Permanent Members

B. Bhakar

Present activities are directed towards the understanding of completely integrable and nonintegrable field theories in low [(1+1) and (2+1)] dimensions. Therefore, investigations are being carried out to study the behaviour of spin chain models on a lattice in (1+1) dimensions with nearest neighbour interactions only. These models are closely related to nonlinear sigma models.

P.G. Blunden

Electromagnetic interactions in complex and few-nucleon systems are being studied. I am particularly interested in the description of electron scattering at large energy and momentum transfers, the so-called quasi-elastic region, in which one or more constituents are knocked out of the nucleus. In this kinematical regime one can explore different aspects of the nuclear response to learn about two-nucleon correlations, two-body electromagnetic currents, the role of nucleon substructure, and the momentum distribution of the initial struck nucleon.

Another area of interest is in a quantum field theory of mesons and hadrons (QHD). Some recent work includes: Dirac-Hartree-Fock calculations for the properties of finite nuclei; hadronic and electromagnetic reactions: a relativistic treatment of mesonic currents; the exact numerical evaluation of one-loop quantum corrections to solitons in 3+1 dimensions; a quark-meson coupling model that treats the nucleon as a collection of confined relativistic quarks embedded in the nuclear medium; and a relativistic mean-field treatment of finite nuclei using light front coordinates.

I have a collaboration with colleagues at Jefferson Lab looking at two-photon exchange corrections in elastic electron-proton scattering. This explanation is a key to resolving a discrepancy between two experimental techniques for extracting the electric and magnetic form factors of the proton at high momentum transfer, and has important implications for our understanding of the structure of the proton.

M.E. Carrington

Finite temperature field theory has applications in many areas. It can be used to study phase transitions like the QCD phase transition in the quark-gluon plasma and the electroweak phase transition in the early universe. It can also be used to study collective behaviour in many body systems, like the production of thermal masses and the propagation of damped plasma oscillations.

It is also of interest to develop calculational techniques to study systems that are not at equilibrium. For example, the lifetime of the quark-gluon plasma is extremely short and it is not clear that there is time to reach equilibrium before the plasma state dissolves. It is likely that an accurate mathematical description of the quark-gluon plasma will involve the use of non-equilibrium methods. Conventional field theoretic techniques assume equilibration, and thus do not apply to unequilibrated systems. There are several methods that can be used to study unequilibrated systems. I am working with transport theory and NPI effective theories.

T. Chakraborty

Spin Transport in a Quantum Dot

It has long been recognized that a two-dimensional electron gas (2DEG) in narrow-gap semiconductors, particularly in InAs-based systems with its high values of the g-factor. exhibit zero-field splitting due to the spin-orbit (SO) coupling. This coupling is also the driving mechanism for making futuristic devices based on controlled spin transport, such as a spin transistor, where the electron spins would precess (due to the SO coupling) while being transported through the 2DEG channel. Tuning of this precession in the proposed spin transistor would provide an additional control that is not available in conventional devices, but may be crucial for the rapidly emerging field of semiconductor spintronics. We have developed a theoretical approach where the SO interaction is treated via exact diagonalization of the Hamiltonian for interacting electrons confined in a parabolic QD. Coulomb interaction causes energy levels to cross and at the crossing point magnetization shows a jump. In an magnetic field the strength of the SO coupling is proportional to the field (in addition to the coupling parameter and the angular momentum). Hence, the effect of the coupling is more prominent for slopes of the higher angular momenta energy curves. As a consequence, an increase in the SO coupling strength causes the energy level crossings to move to weaker fields and the jump in magnetization shows a large shift to weaker magnetic fields. This result can be exploited to tune the SO coupling strength that might be useful for spin transport.

Electron Dynamics in a DNA Molecule

The unique properties of DNA, self-assembly and molecular recognition, has rendered the 'molecule of life' a promising candidate in the rapidly emerging field of molecular nano-electronics. A recent report of a field-effect transistor based on DNA molecules. that was preceded by a series of seminal experiments on the electron conduction in DNA. has sparked a lot of interest on the electronic properties of the DNA. A thorough understanding of the electronic properties of DNA is crucial in the development of the future DNA-based nanoscale devices. In addition, charge transfer through DNA also plays an important role in radiation damage and repair and therefore important for biological processes. We have preformed theoretical calculations of the electron energy spectrum, based on a two-leg charge ladder model for the poly(dA)-poly(dT) DNA and poly(dG)poly(dC) DNA molecules. We take the electron-electron interactions and the electron spin degree of freedom fully into account in our model. The energy spectra for the G-C and the A-T base pairs show a large gap and the interaction was found to enhance the gap. The effect of interaction is less pronounced for the G-C base pairs than that of the A-T pairs. The spin-flip excitations are not the lowest energy excitations. We also analyze the charge distribution for the ground state as well as for the excitations.

J.D. Fiege

This research program explores topics in submillimetre astronomy, planetary science and the interstellar media of other galaxies. The common thread connecting these projects is that they all use computational techniques based on advanced genetic algorithms to explore and test theoretical models using large astronomical data sets. Genetic algorithms are computational techniques for parameter search and optimization that operate in analogy to biological evolution. The author of this proposal previously developed a genetic algorithm called "Ferret" with features designed for difficult data-modeling problems in astrophysics and other physical sciences.

Stars form in dense cores and filaments within molecular clouds. These clouds emit partially polarized submillimetre radiation from dust grains that are aligned perpendicular to the magnetic field, on average. The total intensity is an indicator of the column depth of the gas. However, the direction of linear polarization and the polarization percentage provide constraints on the structure of the magnetic field, which plays a crucial role in the support of molecular clouds against self-gravity, their internal turbulence, and star formation processes. One project uses Ferret to fit theoretical models of magnetized cores and filaments to continuum intensity and polarization data, in order to understand the physics of these objects.

Another project couples Ferret to a planetary structure code to model the internal structure of the moons of Jupiter and Saturn, using constraints from NASA's Galileo Orbiter and the Cassini mission. Three of Jupiter's moons, namely Europa. Callisto and Ganymede, are particularly interesting because they harbour electrically conducting oceans of liquid saltwater beneath a crust of water ice, which interact with Jupiter's magnetosphere to generate magnetic fields. This work is expected to provide improved constraints on the physical conditions within these satellites.

A third project applies Ferret to the task of building global, empirical models of the neutral atomic hydrogen (HI) present in disk galaxies. This phase of the interstellar medium is distributed in a thin disk. We determine the global density, velocity and temperature structure of HI disks, and compare the results for a selection of galaxies.

T.D. Fugleberg

My current research interests have to do with matter and quantum fields under extreme conditions.

I am studying a new state of matter - the colour superconducting state - which may be present in neutron and/or quark stars with consequences detectable in astronomical observations. The colour superconducting state arises in the theory of the strong nuclear force. Quantum Chromodynamics, (QCD). My research involves refining models used in this analysis to include the physical masses of the quarks and other degrees of freedom in as complete a way as possible in order to make definitive quantitative predictions for observation. This research involves free colour charge and is thus related to the main unsolved problem of QCD - colour confinement.

I am also doing research in the areas of non-equilibrium and thermal field theory. Both of these topics have important applications in the physics of the early universe and in heavy ion collisions. I am developing techniques for simplifying calculations in the real time formalism of thermal field theory. Non-equilibrium field theory is still in its infancy but has important implications in the search for the quark gluon plasma and the evolution of the universe immediately following the big bang. I am performing numerical studies of ϕ^4 theory in the 2PPI model in order to understand how quantum fields evolve for arbitrary non-equilibrium initial conditions.

R.L. Kobes

I have three main areas of research interests: quantum field theory, especially at finite temperature and density, classical theories which exhibit chaotic and fractal behaviour, and quantum computing and quantum information theory. Many of the problems we study in these areas involve numerical studies.

G. Kunstatter

Gauge theories provide the theoretical basis for virtually all phenomenological descriptions of the fundamental interactions. They are also playing an increasingly important role in our understanding of certain condensed matter systems. The quantization of gauge theories is, however, complicated by the presence of unphysical modes in the classical description, which must be factored out in order to expose the true physical content of the theory. My research uses geometrical techniques to investigate questions concerning gauge dependence in quantized gauge theories such as Quantum Chromodynamics, Chern-Simons theory and Quantum Gravity, both at zero and finite temperature. Most recently, I have been examining the quantum mechanical behaviour of black holes via simplified field theoretic models in two spacetime dimensions. These models are ideal theoretical

laboratories for the study of fundamental issues surrounding black hole evaporation, such as the statistical mechanical source of entropy and the endpoint of gravitational collapse.

P.D. Loly

In my continuing study of the scientific properties of magical squares a couple of surprising developments have been made recently regarding extensions to my paper with Wayne Chan on compounding magic squares. In essence compounding is an old Chinese idea (before 1275 CE) wherein a base square is incremented and placed in the positions of elements of a frame square. Identical squares may be said to generate "fractal" squares, i.e. self-similar on different scales. Chan and Loly developed a computer implementation of this idea and demonstrated its utility in forging a new world record for large magic squares (order 12,544). In retrospect, perhaps the most important conclusion is that compounding preserves pandiagonality. Now, during the course of preparing a manuscript based on his 2003 summer work, Matt Rempel has developed a remarkable proof of the preservation of the multimagic property (remaining magic after all their elements are raised to a power of 2 or 3 or more, as suggested by Wayne Chan in 2003) of certain magic squares after compounding. Adam Rogers has now been able to show which eigenvalues of compounded magic squares are non-zero on the basis of the eigenvalues of their constituents. He is collaborating with Dan Schindel on these eigenproperties. Studies of the eigenproperties of magic squares have matured to encompass all in fourth order, and to begin to classify the 275 million in fifth order. My study with Daniel Schindel on singular associative (regular) magic squares, the most complete study of eigenproperties of any class of magic squares, is almost finished and we have enlisted the collaboration of Walter Trump (Nuremburg) to incorporate all singular ultramagic squares in seventh order. Schindel, Rempel and I have recently succeeded in counting the number of Benjamin Franklin's bent diagonal squares in eighth order, for which a recent study had given a very large upper bound. This is highly topical with respect to polyhedral cone counting methods, and may well lead to some involvement with the 2006 Franklin anniversary celebrations.

T.A. Osborn

My research program aims to achieve a unification of classical and quantum mechanics in a common mathematical framework. The theory that emerges (quantum phase space, QPS) is an altered version of classical phase space in which the usual commutative product of functions is deformed (as Planck's constant varies away from zero) into a noncommutative (star) product. With this one structural modification it is possible to state the full content of quantum mechanics as a noncommutative phase space theory. In this setting, the Schrödinger wave function never arises. Hilbert space operators are represented by phase space (Wigner) distributions, and quantum expectation values are given by integrals over phase space. This unification via QPS provides an alternate, autonomous statement of quantum mechanics that clarifies its content and interpretation and at the same provides a new computational platform that has many parallels to that of classical mechanics.

Two active projects are: 1) In recent work on charged particle systems in electromagnetic fields we have developed a QPS representation (called a perfect quantization) that is both gauge and geometrically covariant and has an exact star product determined by

a symplectic area phase. Perfect quantization provides an ideal platform for studying the semiclassical charged particle dynamics. We aim to extend this perfect quantization to general non-Abelian gauge theories, i.e., to include Riemannian manifolds and arbitrary spin structure. 2) Develop effective methods to treat long time dynamics in QPS. Rigorously define quantum chaos and the quantum Lyapunov exponent. Investigate the role of the Heisenberg uncertainty principle in the suppression of quantum chaos effects.

B.W. Southern

Statistical Physics

Cooperative phenomena in systems with competing interactions and disorder is a topic of active study. Disorder can arise in many ways such as the dilution of nonmagnetic materials with magnetic impurities or from the loss of perfect translational order in a solid. In particular, in magnetic systems, this competition can arise from the fact that the exchange interaction between magnetic atoms oscillates with distance. If the atoms are located at the sites of a regular lattice, a state of long ranged magnetic order often occurs. However, if there is some disorder in the positions of the atoms, conflicting messages from neighbouring atoms can destroy or weaken this order. In some cases, even if the atoms are arranged so that they lie at the sites of a regular lattice and the interactions are all of the same sign but negative, the order can be weakened to such an extent that the directions of the magnetic moments at zero temperature become completely random. Such systems are said to be frustrated because of the competing interactions and, in this latter case, we refer to the system as geometrically frustrated. Frustration can lead to novel ground states and can change the nature of the excitations in the system. In particular, it can change the nature of topological defects present in the system. These topological defects can interact and exhibit nontrivial unbinding transitions as the temperature increases. Our understanding of these effects is far from complete. A variety of theoretical techniques are employed to study these systems including renormalization group methods. low temperature series methods and numerical Monte Carlo methods.

J. P. Svenne

Our current work has two main themes. The first, and currently most active one, involves work with a multi-channel algebraic system (MCAS) to study scattering of nucleons from light nuclei, and reactions initiated by such. This is a three-continent collaboration with Drs. L. Canton. G. Pisent (Padova University, Italy) and K. Amos. S. Karataglidis and D. van der Knijff (Melbourne University, Australia). The theory uses expansions in Sturmian functions of the channel-coupling interactions, leading to an algebraic solution of the coupled integral equations of the multichannel problem. This enables us to allow for the Pauli principle in the context of a collective model description of the target nucleus, by the use of orthogonalizing pseudo-potentials. The algebraic solution provides us a method of locating all resonances, no matter how narrow, as well as all bound states of the compound system, without the use of an excessively fine energy step sizes. Satisfying the Pauli principle is an essential aspect of the theory, as it removes any spuriosity, in both bound states and resonances and thus provides a theoretical formulation of the scattering

problem that has predictive power. The results of the calculations can also be used to give accurate interpretation of the nuclear structure of the target nucleus and the compound system. Our first work was on the well-studied, both theoretically and experimentally nucleus ¹²C, with scattering by both neutrons and protons, with inclusion of the Coulomb force. The results compare very well with experiment. We are now working on other light and medium mass nuclear systems including systems well away from the valley of stability. Some very exciting new results near the proton drip line have already been obtained and are submitted for publication.

The second theme, in collaboration with L. Canton and G. Pisent at Padua University, focuses on pion absorption on very light nuclei. We have been carrying out practical calculations on 3H and 3He , initially with two-cluster final states: later three-nucleon final states will also be included. This uses various mechanisms and input on πN , NN and $\pi N\Delta$ interactions. The three-nucleon system is treated exactly in a Faddeev-based theory. Final-state interactions are correctly taken into account. In addition to the dominant Δ rescattering contribution to pion production, various other mechanisms, important especially near threshold, are also included. We are able to calculate, along with differential and total cross sections, all possible spin observables, measured or, as yet, not. Comparison with data, where available, is now very good. This work is continuing, and a large paper collecting our main results to date is in preparation.

J.M. Vail

My research is concerned with developing and applying methods to simulate the properties of solid materials. Reliable simulation is an important complement to experiment in studying material properties where subtle variations of chemical composition, crystal structure, electronic configuration, and disorder are crucial, or where time scales, and temperature and pressure regimes are experimentally inaccessible. In 1984, with collaborators, we made a major advance in the atomistic simulation of point defects in ionic materials by combining accurate electronic structure methods for the defect with total energy analysis of the crystal. The method includes physically consistent boundary conditions, the quantum-mechanical ion-size effect, and lattice distortion and polarization, and is embodied in an automated user-friendly program. The method has been applied to charge state and structural stability of defect complexes, optical and spin resonance properties of color centers and impurities, local modification of valence and conduction band edges by impurities, derivation of effective interatomic forces, hole trapping and electron loss by impurities in oxides, local phonon mode frequencies, and classical and quantum diffusion.

Two research projects are current: (1) optical transitions between the electronic state localized at the angstrom level and a state localized at the nanometer level: (2) point-defect properties of group III nitrides.

D.W. Vincent

My general research interests lie in gravitation theory and early universe cosmology. I am currently involved with calculations on multidimensional cosmology solutions of Einstein's

equations, which have relevance to the cosmological constant problem, the Anthropic Principle, and the Many-Worlds approach to quantum cosmology.

J.G. Williams

One of the developing trends in general relativity has been the interest in global, as opposed to local, properties of spacetime. My current research is concerned with spacetimes admitting gravity kinks, i.e. light cone configurations for which the cones tip over an integral number of times. Progress to date includes a kink classification for noncompact product spacetimes in both 3+1 and 2+1 dimensions and the construction of a covariant kink counting number formula in 1+1 dimensions that is related to the Gauss-Bonnet theorem and Morse's Law of Vector Fields. The problem of geodesic incompleteness in spherically symmetric kink spacetimes has been studied in relation to the weak and strong energy conditions, and null geodesics in a number of such spacetimes have been completed using the Kruskal technique. In 2+1 dimensions, a kink solution has been found for the Einstein equations with a perfect fluid source. The mass density, pressure and curvature are all well behaved and the vorticity is nonzero. Future effort will be directed towards introducing time-dependence and to studying the properties of scalar fields in such nonglobally hyperbolic spacetimes.

M. Whitmore

My research group does theoretical studies of soft condensed matter systems, in particular inhomogeneous copolymer systems and phospholipid membranes. Both these classes of molecules have relatively high molecular weights, have chemically distinct sections, and are chain-like in structure. They can self-assemble to form complex nano-scale structures. and undergo subtle phase transitions. A related system is the end-tethered polymer layer, which consists of polymers with one end anchored to a surface, all immersed in solvent. These systems are of wide interest in materials science and biological systems. Our primary goal is to understand them at a fundamental level, primarily using computer-intensive numerical simulations, augmented by relatively simple theories to highlight the underlying physics.

In the area of polymers, our primary focus is on the self-assembly of copolymers, the structures that form, the effects of additives, and the structure of end-tethered polymers. For example, we use numerical self-consistent field (NSCF) theory to calculate the phase diagrams of copolymers and copolymer/solvent blends. Recently, we have been working with chemists at the University of Toronto to understand detailed structural properties of copolymer/homopolymer blends that are observed there. The end-tethered polymer system illustrates the advantages of the NSCF approach. At high molecular weight and tethering density, the molecules become highly stretched, and the system reaches a limit known as the "polymer brush". There exist theories that describe this limit, but it has not been known at what point it is reached. In fact, it is now becoming clear that most systems that are created in the laboratory fall outside this limit. The NSCF theory gives results that are in excellent agreement with recent systematic experiments, identify the onset of the brush limit, and provide a new physical picture of the laboratory systems. Because the NSCF theory is a mean field theory, we have also done Monte Carlo simulations of

many of these systems. They can also be used to construct visual pictures and movies which can provide considerable physical insight. Very recently, we have begun to extend the NSCF theory to incorporate fluctuation effects, in an attempt to understand a long-standing disagreement between theory and experiment near a mean-field critical point in the phase diagram of block copolymers.

My colleague John Whitehead and I have developed an NSCF theory of phospholipid membranes. It provides a detailed picture of these systems, including a range of their structural and thermodynamic properties and their phase behaviour. It is the first theory of its kind to predict effects of pressure which are in good agreement with experiment. In particular, it predicts that the application of hydrostatic pressure causes the layer thickness to increase, rather than decrease as one might expect. We are currently extending this work to mixtures of lipids of different lengths.

4 Research Activities

4.1 Seminars

Date	Speaker	Institution	Title
September 17, 2004	Ken Amos	University of Melbourne, Australia	On new developments in analyses
Jan. 22, 2004	Prof. T. Chakraborty	University of Manitoba	Spintronics: Quantum Mechanics Spin Transitor
April 15, 2004	Dr. A. Barvinsky	Lebedev Physical Institute	Cosmological Constant Problem a Distance Modifications of Einstein
Sept. 27, 2004	Prof. V. Mandelzweig	Racah Institute of Physics	Quasilinearization Method and its Application to Physical Problems

4.2 Visiting Scientists

Dates	Visitor	Institution	
Sept. 16-21, 2004	Ken Amos	University of Melbourne, Australia	
July 8 - Aug. 1, 2005	Luciano Canton	Padova, Italy	

4.3 Graduate Degrees Supervised

- 1. J. Medved (2000). "Thermodynamics of Charged Black Holes in Two-Dimensional Gravity". Ph.D. thesis, University of Manitoba, 2001. (University Microfilms), (Kunstatter).
- 2. S. Peles (2001). "Nonlinear Phenomena and Chaos in Periodically Driven Classical Systems". Ph.D. thesis, University of Manitoba, 2001. (University Microfilms). (Kobes).
- 3. T. Melde (2001). "The Three Nucleon System including one Dynamical Pion: A one dimensional test case". Ph.D. thesis. University of Manitoba, May 2001. (University Microfilms). (Svenne).
- 4. A. Peles (2004). "Frustrated Magnets: A Monte Carlo Study of Stiffness. Vorticity and Topological Excitations". Ph.D. thesis. University of Manitoba. 2004. (University Microfilms), (Southern).
- 5. A. J. Penner (2004). "Nonlinear Analysis of Complicated Physical Systems", MSc thesis. (Kobes).
- 6. S. Barkanova (2004). "The Electroweak Radiative Corrections and Parity-Violating Electron-Nucleon Scattering". PhD thesis, (Blunden).

4.4 Publications of Associate Members/Graduate Students

S. Bekhechi

- 1. S. Bekhechi and B.W. Southern, "Chiral mixed phase in disordered 3d Heisenberg models", *Phys. Rev.* B70, 020405(R) (2004).
- 2. N. Moussa and S. Bekhechi. 'Surface Critical Behavior of Thin Ising Films at the "Special Point" ', *Physica A* 320, 435 (2003).
- 3. S. Bekhechi and B.W. Southern, 'Damage Spreading in Two-Dimensional geometrically frustrated lattices: the triangular and kagome anisotropic Heisenberg model'. J. Phys. A: Math. Gen.36 . 8549 (2003).
- 4. S. Bekhechi and B. W. Southern. 'Off-equilibrium study of the fluctuation-dissipation relation in the easy-axis Heisenberg antiferromagnet on the kagome lattice', *Phys. Rev.* B67. 212406 (2003).
- S. Bekhechi and B.W. Southern, 'Low Temperature Static and Dynamic Behaviour of the Easy-Axis Heisenberg Antiferromagnet on the Kagome Lattice', *Phys. Rev.* B67, 144403 (2003).

A. Borodich

- 1. A.I. Borodich and G.M. Ullmann. Internal hydration of protein cavities: studies on BPTI. Physical Chemistry Chemical Physics. 6:1906-1911 (2004).
- A. Borodich, I. Rojdestvenski, M.G.Cottam, J. Anderson, and G. Oquist. Segregation of the photosystems in higher plant thylakoids and short-term and long-term regulations by a mesoscopic approach. Journal of Theoretical Biology. 225:431-441 (2003).
- A. Borodich, I. Rojdestvenski, M.G. Cottam, and G. Oquist. Segregation of photosystems in thylakoids depends on their size. Biochimica et Biophysica Acta (Bioenergetics) 1606:73-82 (2003).
- 4. A. Borodich, I. Rojdestvenski, and M.G. Cottam. Lateral heterogeneity of photosystems in thylakoid membranes studied by Brownian Dynamics simulations. Biophysical Journal. 85:774-789 (2003).
- I. Rojdestvenski, A.G. Ivanov. M.G. Cottam, A. Borodich, N.P.A. Huner, and G. Oquist. Segregation of photosystems in thylakoid membranes as a critical phenomenon. Biophysical Journal. 82:1719-1730 (2002).

Conference Proceedings

- 6. A. Borodich, I. Rojdestvenski, J. Anderson, and G. Oquist. Segregation of the Photosystems and Short-Term and Long-Term Regulations in Higher Plant Thylakoids. The Sixth Nordic Congress on Photosynthesis. Umea. Sweden. p.14. (2002).
- 7. A. Borodich, I. Rojdestvenski. Segregation of Photosystems in Photosynthetic Membrane of Green Plants. EURESCO conference ce Computational Biophysics:Integrating Theoretical Physics and Biology. San Feliu de Guixols. Spain. p. 58. (2002).
- 8. A.I. Borodich. Transverse Nonlinear Focusing of Nonstationary Space Charge Dominated Beams. Proceedings Of The 1999 Particle Accelerator Conference. N.Y. p. 1869-1871. (1999).
- A.I. Borodich, I.A. Volkov. Optimal Transport of Nonstationary High Intensity Beams. Proceedings Of The 1999 Particle Accelerator Conference. N.Y. p 1872-1874. (1999).

M. Califano

- 1. M. Califano, G. Bester and A. Zunger. "Prediction of a shape-induced enhancement in the hole relaxation in nanocrystals." Nano Lett. 3. 1197 (2003).
- M. Califano and P. Harrison, "Composition, volume and aspect ratio dependence of the strain distribution, band lineups and electron effective masses in self-assembled pyramidal In1-xGaxAs/GaAs and SixGe1-x/Si quantum dots." J. Appl. Phys. 91, 389 (2002).

- 3. M. Califano and P. Harrison. "Quantum box energies as a route to the ground state levels of self-assembled InAs pyramidal dots." J. Appl. Phys. 88, 5870 (2000).
- 4. M. Califano and P. Harrison, "Presentation and experimental validation of a single-band, constant-potential model for self-assembled InAs/GaAs quantum dots." Phys. Rev. B 61, 10959 (2000).
- 5. M. Califano and P. Harrison, "Approximate methods for the solution of quantum wires and dots: Connection rules between pyramidal, cuboidal and cubic dots." J. Appl. Phys. 86, 5054 (1999).

Conference Proceedings

- M. Califano and A. Zunger." Pseudopotential theory of electronic processes in colloidal CdSe quantum dots." Proceedings of the American Chemical Society Meeting 2003. March 23-27. 2003, New Orleans, LA (USA).
- M. Califano, A. Zunger and A. Franceschetti, "Impact ionization in CdSe dots." Proceedings of the 27th International Conference on the Physics of Semiconductors (ICPS2004), July 26-30, 2004. Flagstaff, AZ (USA).
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- 15. M. Pépin, M. D. Whitmore and G. Slater, *Monte Carlo Simulations of Polymers in Solution*, Presented at High Performance Computing Symposium, (HPCS'99), Kingston, ON (2000).
- 16. M. Pépin and M.D. Whitmore, *Optimizing Monte Carlo Simulations of Polymer Systems*. Presented at High Performance Computing Symposium (HPCS'98). Edmonton, AB (1998).
 - **Book Chapters**
- M. D. Whitmore, Block Copolymer Phase Behavior, in Encyclopedia of Materials: Science and Technology. T. P. Lodge, section editor. Elsevier Science Ltd., 657-667 (2001)
- 18. M. D. Whitmore. Theory of Block Copolymers, to appear in Supramolecular Polymers, 2nd edition. A. Ciferri, editor, Marcel Dekker.

Invited Presentations

- 19. M. D. Whitmore, *Modelling and Simulations of Self-Assembly of Block Copolymers*. High Performance Computing Systems and Applications (HPCS '02), Moncton, New Brunswick (2002).
- 20. M. D. Whitmore, Self-Consistent Field Theory of Phospholipid Membranes, Canadian Association of Physicists Congress, Toronto. (June. 2000).
- 21. M. D. Whitmore, *ACEnet: Transforming Research in Atlantic Canada*, High Performance Computing Systems and Applications (HPCS '04), Winnipeg, Manitoba, (May. 2004).
- 22. M. D. Whitmore, *High Performance Computing: The New and Growing Environment in Canada*. Canadian Association of Physicists Congress. Winnipeg. Manitoba (June, 2004).

Contributed Presentations

- 23. I. Mahmoud Abu-Amajieh and M. D. Whitmore, An Examination of the Surface-Pressure Isotherms in End-Tethered Polymer Layers, C.A.P. Congress, Charlottetown, PEI (2003).
- 24. M.D. Whitmore, Experimental and Theoretical Behaviour of End-tethered Polymers from the Mushroom to the Brush Limits, Frontis Symposium on Chain Molecules at Interfaces: SCF Theory and Experiments, Wageningen, the Netherlands (2002).
- 25. M. Pépin and M. D. Whitmore, Characterization of the Surface Density of Endtethered Polymers from the Mushroom to the Brush Limits, Pacifichem 2000 Meeting. Hawaii, (2000).
- 26. M. S. Kent, M. Pépin, J. Douglas and M. D. Whitmore. Experimental and Theoretical Study of End-tethered Ploymers in Good and ⊖ Solvents: Crossover Between the "Mushroom" and "Brush" Limits, A.P.S. March Meeting, Minneapolis, MN (2000).
- 27. M. Pépin and M.D. Whitmore, Relaxation Times and Phase Behaviour in Dilute Copolymer/Homopolymer/Solvent Blends. C.A.P. Congress, Waterloo, ON (1998).

5 Financial

5.1 Statement of Income and Expenditures

Income

Income Source	Amount
Carry over from Aug. 31, 2003	\$4910.00
Total Funds Available	\$4910.00

Expenditures

Activity	Particulars	Amount Spent
Seminars	M. Karasev, Oct. 2003	\$1.000.00
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	V. Vorobiev, Nov. 2003	\$541.08
	A. Barvinsky, April 2004	\$825.41
	Total Visitor Costs	\$2366.49
Miscellaneous	FAX, mail. printing, supplies	\$69.18
	Total Expenditures (2003-2004)	\$2.366.49

In relation to the supporting funds indicated above, it should be pointed out that the members of the Institute use their individual NSERC grants to subsidize Institute activities. Currently the members from the three universities draw upon more than \$250,000 (update) of individual NSERC Research Grants. These funds have a significant fortifying effect on the level of activities in which we are able to engage. The financial contribution of the members associated with the expenses of visiting guest theorists, supports the activities and goals of the Institute, but does not appear in the budget data shown above.

The Institute has neither endowment nor trust fund support. The Institute has no significant space requirements. The occasional long term visitor requires a desk, but these needs have been accommodated by the space available to the physics departments at the member Universities. The host departments also supply occasional secretarial support such as that required for the preparation of seminar notices and research papers.

5.2 Financial Stability and Growth

The Institute has no substantial fixed costs and for this reason it is intrinsically stable. It can operate in a productive fashion at a variety of funding levels. All of the funds that the Institute receives are transformed directly into its research enhancing activities. The funds allocated to the Institute by supportive administrative bodies such as the Faculties of Science and Graduate Studies at the University of Manitoba are fortified

by the individual NSERC research grants of members. This is a strong commitment to the Institute by the Institute members. In view of its overall research productivity, in terms of published papers and supervised graduate students, its capacity for running very successful conferences and workshops, and the demonstrated ability to attract excellent short-term and long-term visiting scientists, the Institute is achieving its goals. The Institute membership includes all of the theoretical physicists in the province. Hence its growth relies solely upon the associate members that it can attract (i.e. graduate students, postdoctoral fellows and research associates). The number and quality of these associate members is dependent on the Institute being able to create a positive research atmosphere. This in turn depends strongly upon the level of funding that the Institute receives. In comparison with its first half dozen years years, in the past six years there has been a marked decrease in the funds made available to the Institute by the three Manitoba universities. This has meant we have not been able to sponsor any costly conferences during this period of time.

The report guidelines suggest that some indication be given of the percentage of time that members spend on Institute research. Since the Institute's programs enhance the ongoing research interests of its members, there is no distinction between individual research and Institute research. The director has spent less than 5% of his time with the administrative aspects of the Institute.