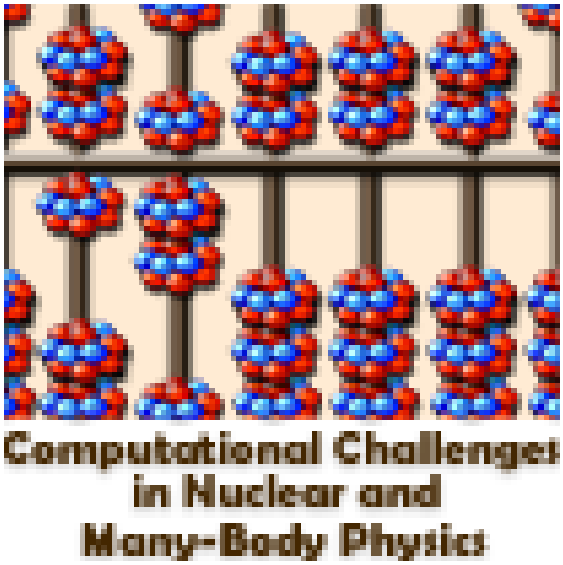
Computational Challenges in Nuclear and Many-Body Physics



Report of Contributions

Contribution ID: **274** Type: **not specified**

New wavefunction forms for strong electron correlation inspired by the eigenvectors of exactly solveable model systems

Modeling strong correlation is so difficult that theorists often settle for qualitative descriptions of strongly-correlated substances (e.g. heavy-fermion materials, high-temperature superconductors). These qualitative approaches are typically based on model Hamiltonians for which the Schrödinger equation can be solved exactly via the Bethe ansatz. We recently realized that one can use the wavefunction-forms from exactly-solvable model Hamiltonians for calculations with the true Hamiltonian (with electrons and nuclei). Choosing a suitable model Hamiltonian ensures that the key qualitative features of the system are all captured, while the computational cost remains low because the exactly solvable model systems can be represented using independent quasiparticles. Our results from wavefunction-forms from the Richardson-Gaudin family of Hamiltonians have remarkable quantitative accuracy: the ground-state energies are typically within 0.001 eV of benchmark results from complete diagonalization in the exponentially big Hilbert space of paired electrons (i.e., doubly-occupied configuration interaction). Using symmetry-broken (unrestricted or general mixed-spin) orbitals to form the Richardson-pairs improves the results still further, and is especially important for spin-frustrated and non-singlet states. The models we present are highly effective for modelling strong correlation, but computationally efficient enough to be applied to large molecules.

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Contribution ID: **275** Type: **not specified**

Exact ground state of strongly correlated electron systems from symmetry-restored wave-functions

The four site Hubbard model is considered from the exact diagonalization and variational method points of view. We show that a symmetry projected mean-field theory recovers the exact ground state energy, irrespective of the interaction strength, in contrast to the conventional Gutzwiller wave-function that will be also considered.

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Contribution ID: **276** Type: **not specified**

Nuclear charge radii of exotic nuclei and superheavy nuclei from the experimental decay data

One of fundamental properties of a nucleus is its radius [1,2]. Experimental information on nuclear charge radii can be obtained by different sources such as electron scattering, muonic atom spectra, isotope shifts, and so on [2,3]. These methods are successful for the nuclei near the beta-stability line. However, it is difficult for them to obtain charge radii of exotic nuclei and superheavy nuclei, because these nuclei are produced by experiments and exhibit short lifetimes so that they are not available as target nuclei. In view of this, we propose a method to determine nuclear charge radii from the decay data [4-8]. As we all know, alpha decay is the main decay mode of heavy and superheavy nuclei [4-6]. We extract their charge radii from the experimental alpha-decay data by the aid of the well-established alpha-decay model [8]. The charge distribution of daughter nuclei is determined in the double-folding model to reproduce the experimental α-decay half-lives. The root-mean-square (rms) charge radius is then calculated using the resulting charge distribution. Nuclear radii of heavy and superheavy nuclei with Z=98-116 are extracted from the alpha-decay data [6-8], for which alpha decay is an unique tool to probe nuclear sizes at present. This is the first result on nuclear charge radii of superheavy nuclei based on the experimental alpha-decay data. Moreover, the rms charge radii of some medium-mass proton-rich nuclei and light neutron-rich nuclei are separately extracted from the experimental data of proton emission and cluster radioactivity in a similar manner [6-8].

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Contribution ID: **277** Type: **not specified**

Studying the density and momentum dependent symmetry energy in a Boltzmann-Langevin approach

Constraining the neutron-proton effective mass splitting is important for extracting the momentum dependencies of the symmetry energy. Within the Boltzmann-Langevin transport model, in which the isospin and momentum-dependent potential is incorporated, we investigate the neutron-proton effective mass splitting in central 112;124;132Sn + 112;124;132Sn collisions at 50 MeV/u. It is found that the transverse momentum, rapidity, and kinetic energy distributions of free neutron over proton ratio are sensitive to the neutron-proton effective mass splitting, especially at higher transverse momenta, at higher kinetic energies, and at larger rapidities. By taking the soft density dependent symmetry energy with the neutron effective mass smaller than that of proton, the calculated results on the double neutron over proton ratios of final free nucleons can reproduce the MSU experimental data.

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Contribution ID: **278** Type: **not specified**

Unconventional Coupled Cluster Theories for Strong and Weak Correlations

Coupled cluster (CC) theory with single and double excitations accurately describes weak electron correlation but is known to fail in cases of strong static correlation. Fascinatingly, however, pair coupled cluster doubles (p-CCD), a simplified version of the theory limited to pair excitations that preserve the seniority of the reference determinant (i.e., the number of unpaired electrons) has mean field computational cost and is an excellent approximation to the full configuration interaction (FCI) of the paired space provided that the orbital basis is optimized to adequately define a pairing scheme. In previous work [1], we have shown that optimization of the pairing scheme in the seniority zero FCI leads to a very accurate description of static correlation. The same conclusion extends to p-CCD [2] if the orbitals are optimized to make the p-CCD energy stationary [3]. The extension of this pair model to quasiparticles will be addressed [4]. We additionally discuss renormalized Hamiltonians via similarity transformation based on Gutzwiller projectors and other exponential forms to describe residual weak correlations [5].

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Contribution ID: **279** Type: **not specified**

Hierarchical Mean-Field Theory

In this talk I present a theoretical framework and a computational method to study the coexistence and competition of thermodynamic phases, and excitations, in strongly correlated quantum Hamiltonian systems. The general framework is known as Hierarchical Mean-Field Theory (HMFT), and its essence revolves around the concept of the relevant elementary degree of freedom (EDOF), e.g., a spin cluster, utilized to build up the system. The system Hamiltonian is then rewritten in terms of these coarse-grained variables and a mean-field (Lie-algebraic) approximation is performed to compute properties of the system. Thus, the (generally) exponentially hard problem of determining, for instance, the ground state of the system is reduced to a polynomially complex one. At the same time, essential quantum correlations, which drive the physics of the problem, are captured by this local representation. Provided the EDOF is chosen properly, even a simple single mean-field approximation, performed on this EDOF, will yield the correct and complete phase diagram, including its phase transition boundaries, {\it in a single computation}. The HMFT predictive power stems from the simple fact that a {\it single} class of states, determined by the EDOF, is used to establish the entire phase diagram of the system. I will describe the zero and finite temperature formulations of the HMFT, and illustrate the plethora of systems where the method has been successfully applied. Examples include frustrated spin systems with exotic magnetic phases, including chiral ones, ring-exchange hard-core boson models, and multiferroics.

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Contribution ID: **280** Type: **not specified**

Microscopic description of nuclear reactions within Coupled Cluster and Gamow Shell Model theories

Nuclei at drip-lines bear unique properties such as halos or resonant character at ground state level, inexistent in the valley of stability. While the latter consists of standard closed quantum systems, drip-line nuclei are open quantum systems, so that models describing their properties must include both nuclear inter-correlations and continuum degrees of freedom. Coupled Cluster and Gamow Shell Model theories, in both ab-initio and effective approaches, are tools of choice for that matter as nuclear correlations are present through configuration mixing while continuum degrees of freedom are imparted by the use of the Berggren basis. The latter methods, initially devised for structure calculations, can now be utilized to study reaction observables. Applications concern direct reactions on light and medium nuclei.

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Presenter: Dr MICHEL, Nicolas (GANIL)

Contribution ID: **281** Type: **not specified**

Coupled channel analysis in nuclear structure

Nuclear structure is better understood in terms of interacting building blocks.
As the first example we discuss the coupled channel Quasiparticle Random Phase Approximation (ccQRPA) for even-even deformed nuclei [1]. The basic building blocks are particle states coupled with the Wigner function to a given total spin.
In this way, we are able to describe collective excitations in deformed nuclei by using building blocks with good angular momentum in the laboratory system.
We obtain a system of coupled QRPA equations with different multipolarities.
An application to E2 transitions shows a significant improvement for the well deformed region in comparison to the standard QRPA. Several applications are proposed.
As a second example we describe electromagnetic and alpha transitions in even-even nuclei by using a common approach for spherical, transitional and deformed nuclei [2].
We use projected coherent states to describe the structure of daugher nuclei and a quadrupole-quadrupole alpha-core interaction to compute decay widths to excited states.
It turns out that the strength of this interaction, reproducing alpha trasitions to 2^+ states, is proportional to the clustering probability. Predictions for electromagnetic
and alpha transitions to excited state are made for all available even-even emitters.
The coupled channel analysis for unfavored alpha transitions in odd mass nuclei is proposed as a promising tool to investigate nuclear structure by the using both spectroscopic and alpha decay data.
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Contribution ID: **282** Type: **not specified**

Algebraically-Stabilized Explicit Integration Of Extremely Stiff Reaction Kinetics Networks with GPU Acceleration

Systems of differential equations containing multiple, widely-separated timescales are termed “stiff”. It is commonly believed that specialized implicit methods must be used to solve such systems because stability limits on the timestep size make standard explicit integration impractical.
This talk will show that even extremely stiff sets of differential equations may be solved efficiently by explicit methods if limiting algebraic solutions are used to stabilize the numerical integration. Employing stringent tests with astrophysical thermonuclear networks, evidence is provided that these methods can deal with the stiffest networks with accuracy and integration timestepping comparable to that of standard implicit methods. Explicit algorithms can execute a timestep faster and scale more favorably with network size than implicit algorithms. Thus, these results suggest that algebraically-stabilized explicit methods might enable integration of much more complex reaction kinetics problems than have been feasible to this point for astrophysics and a variety of other disciplines. Recently we have implemented these new methods on Graphical Processing Unit (GPU) accelerators for large supercomputers such as Titan at ORNL, which permit many such networks to be integrated in parallel. Initial tests for the Type Ia supernova problem suggest that for realistic (hundreds of isotopes) thermonuclear networks these methods can integrate a single network 5-10 times faster than implicit methods, and can integrate of order 100 networks from different zones of the hydro simulation on a single GPU in the same length of time required to integrate a single such network using traditional implicit methods on a CPU. This implies that many problems in a variety of disciplines such as astrophysics, atmospheric and climate science, fission and fusion energy, and combustion chemistry that were previously thought not possible to solve with realistic kinetic networks may now be accessible to these new algorithms deployed on modern computational hardware.

Primary author: Prof. GUIDRY, Mike (University of Tennessee and Oak Ridge National Laboratory)

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Contribution ID: **283** Type: **not specified**

Nuclear Forces and Exotic Oxygen and Calcium Isotopes

Within the context of valence-space Hamiltonians derived from different ab initio many-body methods, I will discuss the importance of 3N forces in understanding and making new discoveries in two of the most exciting regions of the nuclear chart: exotic oxygen and calcium isotopes. Beginning in oxygen, we find that the effects of 3N forces are decisive in explaining why 24O is the last bound oxygen isotope [1,2]. Furthermore, 3N forces play a key role in reproducing spectra, including signatures of doubly magic 22,24O, as well as properties of isotopes beyond the dripline. The calcium isotopes, with potentially three new magic numbers beyond the standard N=20,28, present a unique laboratory to study the evolution of shell structure in medium-mass nuclei. From the viewpoint of two-neutron separation energies and spectroscopic signatures of doubly-magic systems, I emphasize the impact of 3N forces in reproducing the N=28 magic number in 48Ca and in predicting properties of 50-56Ca, which indicate new N=32,34 magic numbers. Finally, I will highlight new efforts to quantify theoretical uncertainties in ab initio calculations of medium-mass nuclei by exploring resolution-scale dependence of observables in sd-shell isotopic/isotonic chains.

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Contribution ID: **284** Type: **not specified**

Beyond-mean-field corrections and effective interactions in the nuclear many- body problem

Mean-field approaches successfully reproduce nuclear bulk properties like masses and radii within the Energy Density Functional (EDF) framework. However, complex correlations are missing in mean-field theories and several observables cannot be predicted accurately. The necessity to provide a precise description of the available data as well as reliable predictions for exotic nuclei motivates the use of sophisticated beyond-mean-field models. A crucial aspect in these calculations is the choice of the effective interaction to be used when one goes beyond the leading mean-field order (available interactions are adjusted at the mean-field level). We have developed techniques to generate new effective interactions that are regularized and are well adapted to be used at a beyond-mean-field level (without double counting problems and divergences). These first studies have been devoted to nuclear matter. Links have been established between the EDF framework and some Effective Field Theory techniques and ideas. The objective of this work is to provide new effective interactions that do not contain any double counting, are cutoff independent, and can be finally used for finite nuclei. This will allow us to perform reliable applications to stable and exotic nuclei with sophisticated beyond-mean-field models.

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Presenter: Dr GRASSO, Marcella (IPN Orsay)

Contribution ID: **285** Type: **not specified**

Superconductivity as a Universal Emergent Phenomenon in Diverse Physical Systems

Superconductivity and superfluidity having generically recognizable features are observed or suspected across a strikingly broad range of physical systems: traditional BCS superconductors, cuprate high-temperature superconductors, iron-based high-temperature superconductors, organic superconductors, heavy-fermion superconductors, and superfluid helium-3 in condensed matter, in many aspects of low-energy nuclear structure physics, and in various exotic possibilities for gravitationally condensed objects such as neutron stars. Microscopically these systems differ fundamentally but the observed superconductivity and superfluidity exhibit two universal features: (1) They result from a condensate of fermion Cooper pairs, and (2) They represent emergent collective behavior that can have only an abstract dependence on the underlying microscopic physics. This universality can hardly be a coincidence but a unified understanding of superconductivity and superfluidity across these highly disparate fields seems impossible microscopically. A unified picture may be possible if superconductivity and superfluidity are viewed as resulting from physics that depends only on broad physical principles operating systematically at the emergent scale, with physics at the underlying microscopic scale entering only parametrically. I will give an overview of superconductivity and superfluidity found in various fermionic condensed matter, nuclear physics, and neutron star systems. I will then propose that all these phenomena result from the systematic occurrence of generic algebraic structures for the emergent effective Hamiltonian, with the underlying microscopic physics being largely irrelevant except for influencing parameter values.

Primary author: Prof. GUIDRY, Mike (University of Tennessee and Oak Ridge National Laboratory)

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Contribution ID: **286** Type: **not specified**

A new approach for large-scale shell-model calculations and large-scale complex scaling calculations

In my presentation, I will present a new approach to numerically solve shell model calculations and complex scaling calculations, which have real energy eigenvalues and complex energy eigenvalues, respectively. For shell model calculations, I have already published in Ref.1 and this new approach works as well as the well-known Lanczos method. In an application concerning to isospin breaking [2], it is superior to the Lanczos method. I will show this new approach in detail.
In the latter part of my presentation, I will show an extension of this work [3] to complex scaling calculations which is useful to describe resonance states. This approach will be able to open large-scale complex scaling calculations.
This work is a result of collaboration with Prof. K. Kaneko, M. Honma, T. Sakurai, Y. Sun, S. Tazaki, G. de Angelis, T. Myo and K. Kato.

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Contribution ID: **287** Type: **not specified**

Temperature dependence of the pair coherence and healing lengths for a fermionic superfluid throughout the BCS-BEC crossover

The pair correlation function and the order parameter correlation function probe, respectively, the intra-pair and inter-pair correlations of a Fermi gas with attractive inter-particle interaction. Here, these correlation functions are calculated in terms of a diagrammatic approach, as a function of coupling throughout the BCS-BEC crossover and of temperature, both in the superfluid and normal phase across the critical temperature T_c. Several physical quantities are obtained from this calculation, including the pair coherence and healing lengths, the Tan's contact, the crossover temperature T^* below which inter-pair correlations begin to build up in the normal phase, and the signature for the disappearance of the underlying Fermi surface which tends to survive in spite of pairing correlations. A connection is also established with experimental data on the temperature dependence of the normal coherence length as extracted from the proximity effect measured in high-temperature (cuprate) superconductors.

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Contribution ID: **289** Type: **not specified**

Nuclear and Particle-Physics Aspects of Condensed-Matter Nanosystems

The physics of condensed-matter nanosystems exhibits remarkable analogies with atomic nuclei. Examples are: Plasmons corresponding to Giant resonances [1], electronic shells, de- formed shapes, and fission [2], beta-type decay, strongly correlated phenomena associated with symmetry breaking and symmetry restoration [3], etc. Most recently, analogies with relativistic quantum-field theories (RQFT) and high-energy particle physics are beeing explored in the field of graphene nanostructures [4].

The talk will review these analogies focusing in particular on the following three aspects:

(1) The shell-correction method (SCM, commonly known as Strutinsky's averaging method and introduced in the 1960's in nuclear physics) was formulated [5] in the context of density functional theory (DFT). Applications of the DFT-SCM (and of a semiempirical variant, SE-SCM, closer to the nuclear Strutinsky approach) to condensed-matter finite systems will be discussed, including the charging and fragmentation of metal clusters, fullerenes, and metallic nanowires [5]. The DFT-SCM offers an improvement compared to the use of Thomas-Fermi gradient expansions for the kinetic energy density functional in the framework of orbital-free DFT.

(2) A unified description of strongly correlated phenomena in finite systems of repelling particles [whether electrons in quantum dots (QDs) or ultracold bosons in rotating traps] has been achieved through a two-step method of symmetry breaking at the unrestricted Hartree- Fock (UHF) level and of subsequent symmetry restoration via post Hartree-Fock projection techniques [3]. The general principles of the two-step method can be traced to nuclear theory (Peierls and Yoccoz) and quantum chemistry (L¨owdin).

This method can describe a wide variety of novel strongly correlated phenomena,
including:
(I) Chemical bonding and dissociation in quantum dot molecules and in single elliptic
QDs, with potential technological applications to solid-state quantum computing.
(II) Particle localization at the vertices of concentric polygonal rings and formation of
rotating (and other less symmetric) Wigner molecules in quantum dots and ultracold
rotating bosonic clouds [6].
(III) At high magnetic field (electrons) or rapid rotation (neutral bosons), the method
yields analytic trial wave functions in the lowest Landau level [7], which are an
alternative to the fractional-quantum-Hall-effect (FQHE) composite-fermion and
Jastrow-Laughlin approaches.
(3) The physics of planar graphene nanorings with armchair edge terminations shows
analo- gies with the physics described by the RQFT Jackiw-Rebbi model and the related
Su-Schrieffer- Heeger model of polyacetylene [4]. This part of the talk will describe the
emergence of exotic states and properties, like solitons, charge fractionization, and
nontrivial topological insulators, in these graphene nanosystems.
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Rev. B 84, 165327 (2011).

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Presenter: Dr YANNOULEAS, Constantine (School of Physics, Georgia Institute of Technology)

Contribution ID: **303** Type: **not specified**

Welcome address

Monday, September 15, 2014 9:30 AM (30 minutes)

Prof. Axel Brandenburg is a member of the Board and Deputy Director of Nordita.

Presenter: BRANDENBURG, Axel

Contribution ID: **304** Type: **not specified**

Defects in Nuclear Pasta

Monday, September 15, 2014 10:00 AM (40 minutes)

Dense nuclear matter, near the base of the crust in neutron stars, is expected to have complex nuclear pasta shapes because of coulomb frustration. Competition between short-range nuclear attraction and long-range coulomb repulsion insures that many different shapes have very similar energies. We report large-scale molecular dynamics simulations of nuclear pasta and find long-lived topological defects. These defects could increase electron pasta scattering and reduce the electrical and thermal conductivities. A reduced thermal conductivity may be visible in X-ray observations of neutron star crust cooling. A reduced electrical conductivity could lead to the decay of magnetic fields.

Presenter: HOROWITZ, Charles

Contribution ID: **305** Type: **not specified**

Coffe break

Contribution ID: **306** Type: **not specified**

Time-Dependent Dynamics of Fermionic Superfluids: from cold atomic gases, to nuclei and neutron stars

The fascinating dynamics of superfluids, often referred to as quantum coherence revealed at macroscopic scale, has challenged both experimentalists and theorists for more than a century now, starting with electron superconductivity discovered in 1911 by Heike Kamerlingh Onnes. The phenomenological two-fluid model of Tizsa and its final formulation due to Landau, is ultimately a classical approach in which Planck's constant never appears and it is unable to describe the generation and dynamics of the quantized vortices, which are the hallmark characteristics of superfluidity.

Various quantum mechanical phenomenological models have been developed over the years by London, Onsager, Feynman, Ginzburg and Landau, Abrikosov, and many others, but truly microscopic approaches are very scarce. The Gross-Pitaevskii equation was for many years the only example, but it is applicable only to a weakly interacting Bose gas at zero temperature and it has been used to describe the large variety of experiments in cold atomic Bose gases. In the case of fermionic superfluids only a time-dependent mean filed approach existed for a long time, which is known to be quite inaccurate. With the emergence of the Density Functional Theory and its time-dependent extension it became relatively recently possible to have a truly microscopic approach of their dynamics, which proves to be extremely relabel in predicting and describing various experimental results in cold atomic fermionic gases, nuclei and which can be used as well to make predictions about the nature and dynamics of vortices in the neutron star crust. I will describe the time-dependent superfluid local density approximation, which is an adiabatic extension of the density functional theory to superfluid Fermi systems and their real-time dynamics.

This new theoretical framework has been used to describe/predict a range of phenomena in cold atomic gases and nuclear collective motion: excitation of the Higgs modes in strongly interacting Fermi superfluids, generation of quantized vortices, crossing and reconnection of vortices, excitation of the superflow at velocities above the critical velocity, excitation of quantum shock waves, domain walls and vortex rings in superfluid atomic clouds, and excitation of collective states in nuclei. This approach is the natural framework to describe in a time-dependent framework various

low energy nuclear reactions and in particular large amplitude collective motion and nuclear fission and the numerical implementation of this formalism requires the largest supercomputers available to science today.

Presenter: BULGAC, Aurel (Seattle, Washington University)

Contribution ID: **307** Type: **not specified**

Nuclear and particle-physics aspects of condensed-matter nanosystems

The physics of condensed-matter nanosystems exhibits remarkable analogies with atomic nuclei. Examples are: Plasmons corresponding to Giant resonances [1], electronic shells, de- formed shapes, and fission [2], beta-type decay, strongly correlated phenomena associated with symmetry breaking and symmetry restoration [3], etc. Most recently, analogies with relativistic quantum-field theories (RQFT) and high-energy particle physics are beeing explored in the field of graphene nanostructures [4]. The talk will review these analogies focusing in particular on the following three aspects: (1) The shell-correction method (SCM, commonly known as Strutinsky's averaging method and introduced in the 1960's in nuclear physics) was formulated [5] in the context of density functional theory (DFT). Applications of the DFT-SCM (and of a semiempirical variant, SE-SCM, closer to the nuclear Strutinsky approach) to condensed-matter finite systems will be discussed, including the charging and fragmentation of metal clusters, fullerenes, and metallic nanowires [5]. The DFT-SCM offers an improvement compared to the use of Thomas- Fermi gradient expansions for the kinetic energy density functional in the framework of orbital-free DFT. (2) A unified description of strongly correlated phenomena in finite systems of repelling particles [whether electrons in quantum dots (QDs) or ultracold bosons in rotating traps] has been achieved through a two-step method of symmetry breaking at the unrestricted Hartree- Fock (UHF) level and of subsequent symmetry restoration via post Hartree-Fock projection techniques [3]. The general principles of the two-step method can be traced to nuclear theory (Peierls and Yoccoz) and quantum chemistry (L¨owdin). This method can describe a wide variety of novel strongly correlated phenomena, including: (I) Chemical bonding and dissociation in quantum dot molecules and in single elliptic QDs, with potential technological applications to solid-state quantum computing. (II) Particle localization at the vertices of concentric polygonal rings and formation of rotating (and other less symmetric) Wigner molecules in quantum dots and ultracold rotating bosonic clouds [6]. (III) At high magnetic field (electrons) or rapid rotation (neutral bosons), the method yields analytic trial wave functions in the lowest Landau level [7], which are an alternative to the fractional-quantum-Hall-effect (FQHE) composite-fermion and

Jastrow-Laughlin approaches. (3) The physics of planar graphene nanorings with armchair edge terminations shows analo- gies with the physics described by the RQFT Jackiw-Rebbi model and the related Su-Schrieffer- Heeger model of polyacetylene [4]. This part of the talk will describe the emergence of exotic states and properties, like solitons, charge fractionization, and nontrivial topological insulators, in these graphene nanosystems. [1] C. Yannouleas, R.A. Broglia, M. Brack, and P.F. Bortignon, Phys. Rev. Lett. 63, 255 (1989); [2] C. Yannouleas, U. Landman, and R.N. Barnett, in Metal Clusters, edited by W. Ekardt (John-Wiley, New York, 1999) Ch. 4, p. 145; [3] C. Yannouleas and U. Landman, Rep. Prog. Phys. 70, 2067 (2007), and references therein; [4] I. Romanovsky, C. Yannouleas, and U. Landman, Phys. Rev. B 87, 165431 (2013); Phys. Rev. B 89, 035432 (2014). [5] C. Yannouleas and U. Landman, Phys. Rev. B 48, 8376 (1993); Ch. 7 in "Recent Advances in Orbital-Free Density Functional Theory," Y.A. Wang and T.A. Wesolowski Eds. (Word Scientific, Singapore, 2013) p. 203 (arXiv:1004.3536); [6] C. Yannouleas and U. Landman, Phys. Rev. Lett. 82, 5325 (1999); I. Romanovsky, C. Yannouleas, and U. Landman, Phys. Rev. Lett. 97, 090401 (2006). [7] C. Yannouleas and U. Landman, Phys. Rev. A 81, 023609 (2010); Phys. Rev. B 84, 165327 (2011).

Presenter: YANNOULEAS, Constantine

Contribution ID: **308** Type: **not specified**

Discussion

Contribution ID: **309** Type: **not specified**

Lunch

Contribution ID: **310** Type: **not specified**

Angular-momentum-projection method to approach nuclear many-body wave functions

In performing shell-model calculations for large nuclear systems, the central issue is how to truncate the shell-model space efficiently. It corresponds to a proper arrangement of the configuration space to separate the most important part from the rest of the space. There are different schemes for the shell-model truncation. Considering the fact that most nuclei in the nuclear chart are deformed, using a deformed basis supplemented by angular momentum projection is an efficient way. Shell-model Hamiltonian is then diagonalized in the projected basis. The method is in principle independent of how a deformed basis is prepared and how an effective interaction is chosen. This approach may be viewed as to bridge the two traditional nuclear physics methods: the deformed mean-field approximation and the conventional shell-model diagonalization, because it keeps all the advantages that a mean-field model has to incorporate important correlations, and has the properties of the conventional shell-model that configurations are mixed beyond the mean-filed states to include effects of residual interactions.
In this talk, we present the above idea by taking the Projected Shell Model and its extensions as examples [1,2,3,4]. Given the strong demand for shell model calculations also from nuclear astrophysics, one needs such an approach that contains sufficient correlations and can generate wave functions in the laboratory frame, thus allowing exact calculations for transition probabilities, spectroscopic factors, and beta-decay and electron-capture rates, in heavy, deformed nuclei.
This research is supported by the National Natural Science Foundation of China (No. 11135005) and by the 973 Program of China (No. 2013CB834401).
[1] K. Hara, Y. Sun, Int. J. Mod. Phys. E4 (1995) 637.
[2] Y. Sun and C.-L. Wu, Phys. Rev. C68 (2003) 024315.
[3] Y. Sun, Int. J. Mod. Phys. E15 (2006) 1695.
[4] Y. Sun, Rev. Mex. Fis. S54(3) (2008) 122

Presenter: SUN, Yang

Contribution ID: **311** Type: **not specified**

Lattice tight-binding Bogoliubov-de Gennes approach to nonuniform superconductivity: Josephson junctions, vortices, and disorder

I will present results on using a lattice tight-binding Bogoliubov-de Gennes formulation of nonuniform superconducting systems and solving self-consistently for the superconducting order parameter. Systems studied include Josephson junctions in graphene and spin-orbit coupled semiconductors, superconducting vortices in spin-orbit coupled semiconductors, and studies of the local effect of impurities and disordered edges in unconventional superconductors. While the method has limitations, especially with regards to system sizes possible to study, it offers a microscopically accurate description of the superconducting state, which can be crucial for a correct physical description of nonuniform superconducting systems.

Presenter: BLACK-SCHAFFER, Annica

Contribution ID: **312** Type: **not specified**

Coffe break

Contribution ID: **313** Type: **not specified**

Hierarchical Mean-Field Theory

In this talk I present a theoretical framework and a computational method to study the coexistence and competition of thermodynamic phases, and excitations, in strongly correlated quantum Hamiltonian systems. The general framework is known as Hierarchical Mean-Field Theory (HMFT), and its essence revolves around the concept of the relevant elementary degree of freedom (EDOF), e.g., a spin cluster, utilized to build up the system. The system Hamiltonian is then rewritten in terms of these coarse-grained variables and a mean-field (Lie-algebraic) approximation is performed to compute properties of the system. Thus, the (generally) exponentially hard problem of determining, for instance, the ground state of the system is reduced to a polynomially complex one. At the same time, essential quantum correlations, which drive the physics of the problem, are captured by this local representation. Provided the EDOF is chosen properly, even a simple single mean-field approximation, performed on this EDOF, will yield the correct and complete phase diagram, including its phase transition boundaries, {\it in a single computation}. The HMFT predictive power stems from the simple fact that a {\it single} class of states, determined by the EDOF, is used to establish the entire phase diagram of the system. I will describe the zero and finite temperature formulations of the HMFT, and illustrate the plethora of systems where the method has been successfully applied. Examples include frustrated spin systems with exotic magnetic phases, including chiral ones, ring-exchange hard-core boson models, and multiferroics.

Presenter: ORTIZ, Gerardo

Contribution ID: **314** Type: **not specified**

Round table

Contribution ID: **315** Type: **not specified**

Low and High-Energy Excitations of the Unitary Fermi Gas

Tuesday, September 16, 2014 9:00 AM (40 minutes)

I describe the use of Quantum Monte Carlo Methods to study low- and high-energy excitations of the Unitary Fermi Gas. We have employed Auxiliary Field Quantum Monte Carlo methods to study this regime of strong pairing in the inhomogeneous gas. The scale invariance of the system places strong constraints on the form of the density functional, unlike nuclear density functionals it can be described in only a very few constants. The derived functional can then be used to predict the properties of small trapped clusters, we find excellent agreement between microscopic calculations of these clusters and results predicted by the density functional. We have also studied the response of the unitary Fermi Gas at very large momentum transfer. Experimentally, the spin and density response are quite different even at very high momentum. We describe approaches to reproduce these responses and analogies to neutrino scattering in nuclei.

Presenter: CARLSON, Joseph

Contribution ID: **316** Type: **not specified**

Quantum simulation of two-dimensional U(1) critical systems: A Higgs particle and the possible help of string theory for the optical conductivity

Tuesday, September 16, 2014 9:40 AM (40 minutes)

Quantum simulators are special purpose devices designed to provide physical insight in a specific quantum problem that is hard to study in the laboratory and impossible on a computer. However, before they can be used they require calibration. For cold atomic systems, quantum Monte Carlo simulations have played a key role there. They established a few years ago that the thermodynamic properties of the experimental system are in one-to-one agreement with the simulations of the corresponding model. The synergy between the two approaches has dramatically progressed since then, to each other's benefice: In the main part of this talk, I will focus on the dynamical properties of a U(1) critical system in (2+1) dimensions focusing on the existence of the amplitude mode or Higgs particle, and on the optical conductivity, which we compare against predictions from the AdS/CFT correspondence. Finally, I will discuss some open problems for this approach to quantum simulation.

Presenter: POLLET, Lode

Contribution ID: **317** Type: **not specified**

Coffe break

Contribution ID: **318** Type: **not specified**

Recent Developments and Applications of the Auxiliary-Field Monte Carlo Method

Tuesday, September 16, 2014 10:40 AM (40 minutes)

The auxiliary-field Monte Carlo (AFMC) method is a powerful technique to calculate thermal and ground-state properties of strongly correlated systems. In particular, it has been extensively applied to study the properties of nuclear and atomic systems. We discuss several recent developments and applications of the method to finite-size systems. (i) In finite systems, it is often necessary to use the canonical ensemble with fixed number of particles. However, the projection on an odd number of particles leads to a new sign problem at low temperatures that has severely limited the application of AFMC to such systems. We discuss a method to circumvent the odd-particle sign problem which allows accurate determination of the ground-state energy, and present its application to the calculation of nuclear pairing gaps from odd-even mass differences [1]. (ii) The level density is among the most important statistical nuclear properties, but its calculation in the presence of correlations is a difficult many-body problem. We discuss recent AFMC calculations of level densities in heavy nuclei. In particular, we present the first microscopic calculation of the collective enhancement factors, which describe the enhancement of level densities by collective states [2]. (iii) Low-temperature calculations require numerical stabilization of the long chains of matrix multiplications necessary to compute the propagator, and a corresponding stabilized method for particle-number projection. The latter is computationally expensive. We discuss an improved method of stabilizing canonical-ensemble calculations that exhibits better scaling and allows calculations for much larger systems [3]. (iv) Deformation is an important concept for the understanding of heavy nuclei. However, it is based on mean-field theory, which breaks rotational invariance, a cornerstone symmetry of finite nuclei. We discuss a method to analyze nuclear deformations at finite temperature using AFMC, which preserves the rotational invariance of the system [4]. In particular, we calculate the probability distribution of the quadrupole operator in heavy rare-earth nuclei, and show that it carries model-independent signatures of deformation. References: [1] A. Mukherjee and Y. Alhassid, Phys. Rev. Lett. 109, 032503 (2012). [2] C. Ozen, Y. Alhassid and H. Nakada, Phys. Rev. Lett. 110,

042502 (2013). [3] C. N. Gilbreth and Y. Alhassid, arXiv:1402.3585 (2014). [4] Y. Alhassid, C. N. Gilbreth and G. F. Bertsch, arXiv:1408.0081 (2014)

Presenter: GILBRETH, Christopher

Contribution ID: **319** Type: **not specified**

TBA

Primary author: DRUT, Joaquin

Contribution ID: **320** Type: **not specified**

Towards the entanglement of strongly coupled fermions via lattice Monte Carlo

Tuesday, September 16, 2014 11:20 AM (40 minutes)

The calculation of the entanglement properties of strongly coupled many-body systems, in particular Renyi and von Neumann entropies, continues to be an active research area with many open questions. In this talk, I will outline the challenges and describe some of the advances, by my group and others, towards the characterization of entanglement in non-relativistic many-fermion systems using novel lattice Monte Carlo strategies.

Presenter: DRUT, Joaquin

Contribution ID: **321** Type: **not specified**

Discussion

Contribution ID: **322** Type: **not specified**

Discussion

Tuesday, September 16, 2014 12:00 PM (1 hour)

Contribution ID: **323** Type: **not specified**

Lunch

Contribution ID: **324** Type: **not specified**

Pfaffians in nuclear structure theory

Tuesday, September 16, 2014 2:30 PM (40 minutes)

In those branches of physics involving quantum many body systems, mean field states are a good starting point for any theoretical study. One of the advantages of mean field states is the existence of generalized Wick theorems that simplify the evaluation of operator overlaps. Unfortunately, the number of terms to be considered increase with the double factorial of the number of creation and annihilation operators in the overlap. This and other problems that appear when the mean field states are of the Hartree Fock Bogoliubov (HFB) type can be easily handled introducing fermion coherent state techniques and the pfaffian. In my talk I will discuss this technique and the applications involving HFB states in the context of symmetry restoration and configuration techniqes common in low energy nuclear structure calculations.

Presenter: ROBLEDO, Luis

Contribution ID: **325** Type: **not specified**

Auxiliary-field calculations with or without the sign problem:from Fermi gases to molecules to solids

Tuesday, September 16, 2014 3:10 PM (40 minutes)

I will describe recent progress in developing a general framework for accurate ground-state calculations of interacting electronic systems. This framework is based on the use of auxiliary-fields, and addresses the sign problem (which turns into a phase problem for realistic electron-electron interactions) by constraining the imaginary-time
paths with an approximate sign (gauge) condition. The approach can be used to study either a fully materials-specific Hamiltonian or a Hubbard-like model — or indeed any electronic Hamiltonian in between as the former is "down-folded" to the latter.
As an example of materials-specific calculations, we determine the equation of state in a variety of solids, which systematically removes deficiencies of density-functional theory (DFT) results. As an example of model studies, the nature of magnetic and charge correlations in the doped Hubbard model are determined, in the context of models for high-temperature superconductivity. Its implications on the search for so-called FFLO phases with cold atoms will be discussed. We also present exact results on the properties of the two-dimensional ultracold Fermi gas. Calculations in systems with strong spin-orbit coupling will be discussed.

Presenter: ZHANG, Shiwei

Contribution ID: **326** Type: **not specified**

Coffe break

Tuesday, September 16, 2014 3:50 PM (20 minutes)

Contribution ID: **327** Type: **not specified**

The isospin- and angular-momentum-projected density functional theory and beyond: formalism and applications

Tuesday, September 16, 2014 4:10 PM (40 minutes)

Over the last few years we have developed the multi-reference density functional theory (DFT) involving the isospin- and angular-momentum projections of a single Slater determinant. The model, dubbed below static, was specifically designed to treat rigorously the conserved rotational symmetry and, at the same time, tackle the explicit breaking of the isospin symmetry resulting from a subtle balance between the long-range isospin-symmetry-breaking Coulomb field and short-range isospin-symmetry-conserving (predominantly) strong force. These unique features allowed us to calculate, in between, the isospin impurities in N˜Z nuclei and isospin symmetry breaking corrections (ISB) to superallowed Fermi beta-decay matrix elements. Recently, we have extended the model to a variant (hereafter called dynamic) that allows for mixing of states that are projected from self-consistent Slater determinants representing low-lying (multi)particle-(multi)hole excitations. The states that are mixed have good angular momentum and, at the same time, include properly treated Coulomb isospin mixing. Hence, the extended model can be considered as a variant of the no core configuration-interaction approach, with two-body short-range (hadronic) and long-range (Coulomb) interactions treated on the same footing. It is based on a truncation scheme dictated by the self-consistent deformed Hartree-Fock (HF) solutions. The model can be used to calculate spectra, transitions, and beta-decay matrix elements in any nuclei, irrespective of their neutron- and proton-number parities. The aim of the talk is to introduce the theoretical frameworks of both the static and dynamic approaches and present selected applications. The applications will be focused on nuclei relevant to high-precision tests of the weak-interaction flavor-mixing sector of the Standard Model. In this context, we will present the results for ISB corrections to superallowed Fermi transitions and for the low-spin spectra in: 32S and 32Cl nuclei, in A=38 Ar, K, and Ca nuclei, and in 62Ga and 62Zn nuclei. In case of 62Zn the spectrum of 0+ states will be addressed. The 0+ states in this nucleus were reassigned in a recent experiment, and are now posing a challenge to theory.

Presenter: SATULA, Wojciech

Contribution ID: **328** Type: **not specified**

Round table

Tuesday, September 16, 2014 4:50 PM (40 minutes)

Contribution ID: **329** Type: **not specified**

Clustering and response functions of light nuclei in explicitly correlated Gaussians

Explicitly correlated Gaussian basis is used for solving few-body problems in many fields. The basis functions are easily adaptable and flexible enough to describe complex few-body dynamics. We obtain a unified description of different types of structure and a fair account of correlated motion of interacting particles as well as the tail of the wave function. I present some examples that show the power of the correlated Gaussians: The bound and resonant states of 4He, the electric dipole response functions of 4He and 6He, and alpha-clustering in 16O in the framework of a 12C core plus four nucleon model.
It is a challenge for future to extend the application of the correlated Gaussians to a study on a competition between single-particle motion and clustering around a non-inert core. Such a study will be important to evaluate the rate of the radiative capture reactions 12C(alpha, gamma)16O at low energy and to account for the low-lying spectrum of 212Po that shows the large alpha-decay width and the enhanced electric dipole transitions.

Presenter: SUZUKI, Yasuyuki

Contribution ID: **330** Type: **not specified**

Clustering and response functions of light nuclei in explicitly correlated Gaussians

Wednesday, September 17, 2014 10:00 AM (40 minutes)

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Presenter: SUZUKI, Yasuyuki

Contribution ID: **331** Type: **not specified**

Superconductivity as a Universal Emergent Phenomenon in Diverse Physical Systems

Wednesday, September 17, 2014 10:40 AM (40 minutes)

Superconductivity and superfluidity having generically recognizabl features are observed or suspected across a strikingly broad range of physical systems: traditional BCS superconductors, cuprate high temperature superconductors, iron-based high-temperature superconductors, organic superconductors, heavy-fermion superconductors, and superfluid helium-3 in condensed matter, in many aspects of low-energy nuclear structure physics, and in various exotic possibilities for gravitationally condensed objects such as neutron stars. Microscopically these systems differ fundamentally but the observed superconductivity and superfluidity exhibit two universal features: (1) They result from a condensate of fermion Cooper pairs, and (2) They represent emergent collective behavior that can have only an abstract dependence on the underlying microscopic physics. This universality can hardly be a coincidence but a unified understanding of superconductivity and superfluidity across these highly disparate fields seems impossible microscopically. A unified picture may be possible if superconductivity and superfluidity are viewed as resulting from physics that depends only on broad physical principles operating systematically at the emergent scale, with physics at the underlying microscopic scale entering only parametrically. I will give an overview of superconductivity and superfluidity found in various fermionic condensed matter, nuclear physics, and neutron star systems. I will then propose that all these phenomena result from the systematic occurrence of generic algebraic structures for the emergent effective Hamiltonian, with the underlying microscopic physics being largely irrelevant except for influencing parameter values.

Presenter: GUIDRY, Mike

Contribution ID: **332** Type: **not specified**

Coffe break

Wednesday, September 17, 2014 11:20 AM (20 minutes)

Contribution ID: **333** Type: **not specified**

No-Core CI calculations of light nuclei: Emergence of rotational bands

Wednesday, September 17, 2014 11:40 AM (40 minutes)

The atomic nucleus is a self-bound system of strongly interacting nucleons. In No-Core Configuration Interaction (CI) calculations, the nuclear wavefunction is expanded in a basis of Slater Determinants of single-nucleon wavefunctions (Configurations), and the many-body Schrödinger equation becomes a large sparse matrix problem. The challenge is to reach numerical convergence to within quantifiable numerical convergence to within quantifiable numerical uncertainties for physical observables using finite truncations of the infinite-dimensional basis space. I discuss the (dis)advantages of different truncation schemes, as well as strategies for constructing and solving the resulting large sparse matrices of current multi-core computer architectures. Several of these strategies have been implemented in the code MFDn, a hybrid MPI/OpenMP Fortran code for ab-initio nuclear structure calculations that has been demonstrated to scale to over 200,000 cores. Finally, I present results for ground state energies, excitation spectra, and select electromagnetic observables for light nuclei in the A=6 to 14 range using realistic 2- and 3-body forces. In particular, I demonstrate that collective phenomena such as rotational band structures can emerge from these microscopic calculations.

Presenter: MARIS, Pieter

Contribution ID: **334** Type: **not specified**

Discussion

Wednesday, September 17, 2014 12:20 PM (40 minutes)

Contribution ID: **335** Type: **not specified**

Lunch

Wednesday, September 17, 2014 1:00 PM (1h 30m)

Contribution ID: **336** Type: **not specified**

A new approach for large-scale shell-model calculations and large-scale complex scaling calculations

Wednesday, September 17, 2014 2:30 PM (40 minutes)

In my presentation, I will present a new approach to numerically solve shell model calculations and complex scaling calculations, which have real energy eigenvalues and complex energy eigenvalues, respectively. For shell model calculations, I have already published in Ref.1 and this new approach works as well as the well-known Lanczos method. In an application concerning to isospin breaking [2], it is superior to the Lanczos method. I will show this new approach in detail. In the latter part of my presentation, I will show an extension of this work [3] to complex scaling calculations which is useful to describe resonance states. This approach will be able to open large-scale complex scaling calculations. This work is a result of collaboration with Prof. K. Kaneko, M. Honma, T. Sakurai, Y. Sun, S. Tazaki, G. de Angelis, T. Myo and K. Kato. Reference [1] T. Mizusaki, K. Kaneko, M. Honma, T. Sakurai, Phys. Rev. C82 024310 (2010). [2] T. Mizusaki, K, Kaneko, M. Honma, K. Sakurai, Acta Phsica Polonica B 42, 447 (2011). K. Kaneko, T. Mizusaki, Y. Sun, S. Tazaki, G. de Angelis, Phys. Rev. Lett. 109, 092504 (2012). [3] T.Mizusaki, T.Myo, K.Kato, to be submitted.

Presenter: MIZUSAKI, Takahiro

Contribution ID: **337** Type: **not specified**

Ab-initio calculations of nuclei with many-body perturbation theory

Wednesday, September 17, 2014 3:10 PM (40 minutes)

We start from a realistic nuclear force (N3LO [1] or JISP16 [2]), and use the similarity renormalization group (SRG) to renormalize the realistic nuclear force. With the softened NN force, we first perform the Hartree-Fock (HF) calculation, and then take the HF solution as the reference and basis for further corrections to the solution of the many-body system. The many-body perturbation theory (MBPT) [3] has been employed for the correction calculations. Corrections up to the third order in energy and up to second order in radius have been considered. As preliminary investigations, we have calculated 4He and 16O, obtaining quite good converged results in their binding energies and radii. We thank J. Vary for providing the JISP16 interaction and useful discussions. [1] D.R. Entem and R. Machleidt, Phys. Rev. C 68, 041001 (32003); [2] A.M. Shirokov, A.I. Mazur, S/A. Zaytsev, J.P. Vary and T.A. Weber, Phys. Rev. C 70, 044005 (2004); [3] I. Shavitt and R.J. Bartlett, Many-body methods in Chemistry and physics: MBPT and coupled-cluster theory (2009).

Presenter: XU, Furong

Contribution ID: **338** Type: **not specified**

Coffe break

Wednesday, September 17, 2014 3:50 PM (20 minutes)

Contribution ID: **339** Type: **not specified**

Neutrino physics and nuclear structure for double-beta decay

Neutrinoless double-beta decay, if observed, would signal physics beyond the Standard Model that would be discovered at energies significantly lower than those at which the relevant degrees of freedom can be excited. Therefore, it could be difficult to use the neutrinoless double-beta decay observations to distinguish between several beyond Standard Model competing mechanisms that were propose to explain this process. Accurate nuclear structure calculations of the nuclear matrix elements (NME)
necessary to analyze the decay rates could be helpful to narrow down the list of competing mechanisms, and to better identify the more exotic properties of the neutrinos. In my talk I will review the neutrino physics relevant for double-beta decay, I will analyze the status of the shell model calculation of the NME, and their relevance for discriminating the contribution of possible competing mechanisms to the neutrinoless double-beta decay process.
U.S. DoE grant DE-SC0008529 and U.S. NSF grants PHY-1068217 and PHY-1404442 are acknowledged.

Presenter: HOROI, Mihai

Contribution ID: **340** Type: **not specified**

Nucleon-pair Approximation of the shell model

Wednesday, September 17, 2014 4:50 PM (40 minutes)

Atomic nuclei are complex systems of protons and neutrons that strongly interact with each other via an attractive and short-range force, leading to a pattern of dominantly monopole and quadrupole correlations between like particles (i.e., proton-proton and neutron-neutron correlations) in low-lying states of atomic nuclei. Among many nucleon pairs, very few nucleon pairs such as proton and neutron pairs with spin zero, two, and occasionally isoscalar proton-neutron pairs with spin aligned, play a dominant role in low-energy nuclear structure. Therefore the nucleon-pair approximation provides us with an efficient truncation scheme of the full shell model configurations which are otherwise too large to handle for medium and heavy nuclei. Furthemore, the nucleon-pair approximation leads to simple pictures in physics, as the dimension of nucleon-pair subspace is small. In this talk I would like to give a brief review of its history, formulation, validity, applications, as well as its link to previous approaches. Numerical calculations of low-lying states for realistic atomic nuclei are demonstrated with examples. Applications of pair approximations to other problems are also discussed.

Presenter: ZHAO, Yu-Min

Contribution ID: **341** Type: **not specified**

Toward model-independent calculations of atomic nuclei

Thursday, September 18, 2014 9:00 AM (40 minutes)

This talk reviews recent results of coupled-cluster calculations for rare isotopes, optimization of interaction from chiral effective field theory, and finite size effects in the oscillator basis.

Presenter: PAPPENBROCK, Thomas

Contribution ID: **342** Type: **not specified**

Highly Frustrated Spin-Lattice Models of Magnetism and Their Quantum Phase Transitions: A Microscopic Treatment via the Coupled Cluster Method

Thursday, September 18, 2014 9:40 AM (40 minutes)

The coupled cluster method [1] (CCM) is one of the most pervasive, most powerful, and most successful of all ab initio formulations of quantum many-body theory. It has probably been applied to more systems in quantum field theory, quantum chemistry, nuclear, subnuclear, condensed matter and other areas of physics than any other competing method. The CCM has yielded numerical results which are among the most accurate available for an incredibly wide range of both finite and extended physical systems defined on a spatial continuum. These range from atoms and molecules of interest in quantum chemistry, where the method has long been the recognized "gold standard", to atomic nuclei; from the electron gas to dense nuclear and baryonic matter; and from models in quantum optics, quantum electronics, and solid-state optoelectronics to field theories of strongly interacting nucleons and pions.

This widespread success for both finite and extended physical systems defined on a spatial continuum [2] has led to recent applications to corresponding quantum-mechanical systems defined on an extended regular spatial lattice.

Such lattice systems are nowadays the subject of intense theoretical study. They include many examples of systems characterized by novel ground states which display quantum order in some region of the Hamiltonian parameter space, delimited by critical values which mark the corresponding quantum phase transitions. The quantum critical phenomena often differ profoundly from their classical counterparts, and the subtle

correlations present usually cannot easily be treated by standard many-body techniques (e.g., perturbation theory or mean-field approximations). A key challenge for modern quantum many-body theory has been to develop microscopic techniques capable of handling both these novel and more traditional systems. Our recent work shows that the CCM is capable of bridging this divide. We have shown how the systematic inclusion of multispin correlations for a wide variety of quantum spin-lattice problems can be efficiently implemented with the CCM [3]. The method is not restricted to bipartite lattices or to non-frustrated systems, and can thus deal with problems where most alternative techniques,

e.g., exact diagonalization of small lattices or quantum Monte Carlo (QMC) simulations, are faced with specific difficulties.
In this talk I describe our recent work that has applied the CCM to strongly interacting and highly frustrated spin-lattice models of interest in quantum magnetism, especially in two spatial dimensions. I show how the CCM may readily be
implemented to high orders in systematically improvable hierarchies of approximations, e.g., in a localized lattice-animal-based subsystem (LSUBm) scheme, by the use of computer-algebraic techniques. Values for ground-state (and excited-state) properties are obtained which are fully competitive with those from other state-of-the-art methods, including the much more computationally intensive QMC techniques in the relatively rare (unfrustrated) cases where the latter can be readily applied. I describe the method itself, and illustrate its ability to give accurate descriptions of the ground-state phase diagrams of a wide variety of frustrated magnetic systems via a number of topical examples of its high-order implementations, from among a very large corpus of results for spin lattices. The raw LSUBm results are themselves generally excellent. I show explicitly both how
they converge rapidly and can also be accurately extrapolated in the truncation index, $m \to \infty$, to the exact limit.
[1] R.F. Bishop, in "Microscopic Quantum Many-Body Theories and Their Applications," (eds. J. Navarro and A. Polls), Lecture Notes in Physics Vol. 510, Springer-Verlag, Berlin (1998), 1.
[2] R.F. Bishop, Theor. Chim. Acta 80 (1991), 95; R.J. Bartlett, J. Phys. Chem. 93 (1989), 1697.
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Presenter: BISHOP, Raymond

Contribution ID: **343** Type: **not specified**

Coffe break

Thursday, September 18, 2014 10:20 AM (20 minutes)

Contribution ID: **344** Type: **not specified**

Open-shell systems via symmetry (broken and) restored coupled cluster theory

Thursday, September 18, 2014 10:40 AM (40 minutes)

Ab initio many-body methods have been developed over the past ten years to address closed-shell nuclei up to mass $A \sim 130$ on the basis of realistic two- and three-nucleon interactions. A current frontier relates to the extension of those many-body methods to the description of open-shell nuclei. Several routes are currently under investigation to do so among which one relies on the powerful concept of spontaneous symmetry breaking. Singly open-shell nuclei can be efficiently described via the breaking of U(1) gauge symmetry associated with particle-number conservation, as a way to account for their superfluid character. Doubly open-shell nuclei can be addressed by further breaking SU(2) symmetry associated with angular momentum conservation. Still, the description of finite quantum systems eventually requires the exact restoration of symmetry quantum numbers. In this context, we discuss two recent developments performed within the frame of single-reference coupled cluster theory. First, we present the Bogoliubov coupled cluster formalism, which consists of representing the exact ground-state wave function of the system as the exponential of a quasi-particle excitation cluster operator acting on a Bogoliubov reference state. Test calculations for the pairing Hamiltonian are presented along with realistic proof-of-principle calculations of even-even nuclei with $A \approx 20$. Second, we discuss a recent extension of symmetry-unrestricted coupled-cluster theory that allows for the exact restoration of the broken symmetry at any truncation order. The formalism, which encompasses both single-reference coupled cluster theory and projected Hartree-Fock theory as particular cases, permits the computation of usual sets of connected diagrams while consistently incorporating static correlations through the highly non-perturbative restoration of the symmetry. A key difficulty relates to the necessity to handle generalized energy {\it and} norm kernels for which naturally terminating coupled-cluster expansions are indeed obtained. The focus is on SU(2) and U(1) symmetries but the formalism can be extended to any (locally) compact Lie group and to discrete groups, such as most point groups.

Presenter: DUGUET, Thomas

Contribution ID: **345** Type: **not specified**

Pairing and quarteting in proton-neutron systems

Thursday, September 18, 2014 11:20 AM (40 minutes)

The common treatment of proton-neutron pairing in N ≅ Z nuclei relies on Cooper pairs and mean-field BCS-type models. However, the nuclear interaction can induce, through the isospin conservation, quartet correlations of alpha type which might compete with the Cooper pairs. In fact, for any isovector pairing interactions the ground state of N=Z systems is accurately described not by Cooper pairs but in terms of collective quartets [1,2]. Cooper pairs and quartets can however coexist in isospin asymmetric systems with N>Z. In this case the ground state of the isovector pairing Hamiltonian can be described with high precision as a condensate of alpha-like quartets to which it is appended a condensate of Cooper pairs built with the excess neutrons [3,4]. Quartets appear to be the relevant degrees of freedom for treating not only the isovector pairing but also the competition between the isoscalar and the isovector proton-neutron pairing in N=Z nuclei [5]. These facts indicate that the many-body pairing problem in N ≅ Z nuclei can be more efficiently treated in calculation schemes based on alpha-type quartets rather than on Cooper pairs and BCS-type models.
1.N. Sandulescu, D. Negrea, J. Dukelski, C. W. Johnson, Phys. Rev. C85, 061303 (R) (2012); 2. N. Sandulescu, D. Negrea, C. W. Johnson, Phys. Rev. C86, 041302 (R) (2012); 3. M. Sambataro and N. Sandulescu, Phys Rev. C88, 061303 (R)(2013) ; 4. D. Negrea and N. Sandulescu, Phys. Rev. C (2014), in press; 5. M. Sambataro, N. Sandulescu and C. W. Johnson, in preparation

Presenter: SANDULESCU, Nicolae

Contribution ID: **346** Type: **not specified**

Discussion

Thursday, September 18, 2014 12:00 PM (1 hour)

Contribution ID: **347** Type: **not specified**

Lunch

Thursday, September 18, 2014 1:00 PM (2 hours)

Contribution ID: **348** Type: **not specified**

Nuclear physics: a laboratory for many-particle quantum mechanics

Presenters: BERTSCH, George; BERTSCH (COLLOQUIUM), George

Contribution ID: **349** Type: **not specified**

Nuclear physics: a laboratory for many-particle quantum mechanics (Colloquium)

Presenter: BERTSCH, George

Contribution ID: **350** Type: **not specified**

Quantum tensor networks for simulating quantum spin systems

Friday, September 19, 2014 9:00 AM (40 minutes)

Presenter: VERSTRAETE, Frank

Contribution ID: **351** Type: **not specified**

Tensor methods and entanglement measurements for models with long-range interactions

Friday, September 19, 2014 9:40 AM (40 minutes)

Strongly correlated materials are typically rather difficult to treat theoretically. They have a complicated band structure, and it is quite difficult to determine which minimal model correctly describes their essential physical properties. Moreover, the value of the model parameters to be used for a given material is often the subject of debate. Unfortunately, analytic approaches often do not provide rigorous conclusions for the interesting parameter sets, therefore, numerical simulations are mandatory.
Momentum-space formulations of local models such as the Hubbard model and problems in quantum chemistry are especially hard to treat using matrix- and tensor product-based algorithms because they contain non-local interactions. Quantum entropy-based measures can be used to map the entanglement structure in order to gain physical information and to optimize algorithms.
In this tutorial contribution, we present an overview of the real space, momentum space and quantum chemistry versions of the DMRG/MPS and tree-TNS algorithms and their applications to various spin and fermionic lattice models, and to transition metal complexes. Data sparse representation of the wavefunction will be investigated through advances in entanglement localization providing optimized tensor topologies. Entropy generation by the RG procedure, the mutual information leading to a multiply connected network of lattice sites or orbitals, and reduction of entanglement by basis transformation will be discussed. Inclusion of the concepts of entanglement will be used to identify the wave vector of soft modes in critical models, to determine highly correlated molecular orbitals leading to an efficient construction of active spaces and for characterizing the various types of correlation effects relevant for chemical bonding.
The state of the art matrix-product-based algorithms is demonstrated on polydiacetylene chains by reproducing experimentally measured quantities with high accuracy.
[1] S. R. White, Phys. Rev. Lett. 69, 2863-2866 (1992).
[2] S. R. White and R. L. Martin, J. Chem. Phys. 110, 4127-4130 (1999).
[3] O. Legeza, R. M. Noack, J. SĂłlyom, and L. Tincani, in Computational Many-Particle Physics, eds. H. Fehske, R.

Schneider, and A. Weisse 739, 653-664 (2008).
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[6] O. Legeza and J. SĂłlyom, Phys. Rev. B 68, 195116 (2003), ibid Phys Rev. B 70, 205118 (2004).
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[8] K. Boguslawski, P. Tecmer, O. Legeza, and M. Reiher, J. Phys. Chem. Lett. 3, 3129-3135 (2012).
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[13] G. Barcza, O. Legeza, K. H. Marti, and M. Reiher, Phys. Rev. A 83, 012508 (2011).
[14] G. Barcza, R. M. Noack, J. SĂłlyom, O. Legeza, arxiv:1406.6643 (2014)

Presenter: LEGEZA, Örs

Contribution ID: **352** Type: **not specified**

Coffe break

Friday, September 19, 2014 10:20 AM (20 minutes)

Contribution ID: **353** Type: **not specified**

Integrable Richardson-Gaudin bases for pairing Hamiltonians

Friday, September 19, 2014 10:40 AM (40 minutes)

Configuration interaction methods for quantum many-body systems are generally represented within Fock space, the space spanned by all possible single-particle Slater determinant (SD) wave functions. For strongly-correlated quantum systems, the number of physically important SD basis states quickly reaches beyond the capacities of present (and future) computer hardware, due to the lack of correlations within these SD basis states. Bases spanned by Richardson-Gaudin (RG) eigenstates can be regarded as a generalisation of Fock space, because the strong correlations are inherently present within the basis states. In this contribution, it will be shown how configuration interaction methods can benefit from the use of RG bases over conventional Fock space.

Presenter: DE BAERDEMACKER, Stijn

Contribution ID: **354** Type: **not specified**

Disorder in bilayer and double layer graphene

Friday, September 19, 2014 11:20 AM (40 minutes)

We use a numerical application of Thomas-Fermi theory to describe the effects of fluctuations in the local charge density caused by charged impurities in bilayer and double layer graphene. In the bilayer, we show that the interplay between the non-linear screening of the disorder potential and a band gap causes the electron liquid to break into coexisting compressible and incompressible regions. For double layer graphene, we demonstrate that charged impurity disorder has
a significant negative impact on the existence of theproposed excitonic condensate.

Presenter: ABERGEL, David

Contribution ID: **355** Type: **not specified**

TBA

Contribution ID: **356** Type: **not specified**

Discussion

Friday, September 19, 2014 12:00 PM (1 hour)

Contribution ID: **357** Type: **not specified**

Lunch

Friday, September 19, 2014 1:00 PM (1h 30m)

Contribution ID: **358** Type: **not specified**

Aspects of time-dependence in many-body systems

Friday, September 19, 2014 2:30 PM (40 minutes)

Dynamical processes set yet another degree of complexity to the many-body problem. With the advent of ultrafast measuring techniques modern experiments often leave the regime of adiabaticity or linear response. The evolution of quantum systems on short time scales subject to strong disturbances then becomes relevant. In this contribution, I will present two different examples that demonstrate aspects of non-equilibrium dynamics in many-body quantum systems. The first example considers the temporal evolution of a closed many-body-system represented by a simple molecule being exposed to a strong ionizing light pulse. Solving the time-dependent Schrödinger equation reveals different processes in the charge dynamics following ionization. It will be demonstrated that a proper choice of electron-hole excitations is crucial for capturing the essential physics. The second example features the non-equilibrium dynamics of an open quantum system. The spin of a magnetic ad-atom residing on the surface of a non-magnetic substrate is exposed to the tunneling current of a scanning tunneling microscope. Spin torque of the tunneling electrons induces spin-dynamics of the surface spin. A master-equation approach is used to solve von-Neumann's equation of motion for the reduced density matrix of the surface spin. Challenges in computing the short time dynamics of the system by different methods are being exhibited.

Presenter: PFANNKUCHE, Daniela

Contribution ID: **359** Type: **not specified**

Path integral simulations of bosons with disorder

Friday, September 19, 2014 3:10 PM (40 minutes)

Monte Carlo simulation of worldlines of quantum particles in a path integral representation is a powerful tool mainly used for studying boson systems. Such approaches have been used to investigate properties of superfluid helium in confined geometries and localization of bosons in a random disorder potential. In particular we are interested in the role of correlations of the disorder distribution. I will introduce theoretical tools and techniques and discuss opportunities, difficulties and challenges in this field.

Presenter: WALLIN, Mats

Contribution ID: **360** Type: **not specified**

Coffe break

Friday, September 19, 2014 3:50 PM (20 minutes)

Contribution ID: **361** Type: **not specified**

Summary

Friday, September 19, 2014 4:10 PM (40 minutes)

Presenter: ALHASSID, Yoram

Contribution ID: **362** Type: **not specified**

Nuclear physics: a laboratory for many-particle quantum mechanics (Colloquium)

Contribution ID: **363** Type: **not specified**

Nuclear physics: a laboratory for many-particle quantum mechanics (Colloquium)

Thursday, September 18, 2014 3:00 PM (1 hour)

Nuclear structure physics has presented a fruitful testing ground for quantum many-body theory since its beginnings half a century ago. On the one hand, the observed phenomena have given rise to models that have been invaluable to interpret the underlying physics. On the other hand, the quest to make a predictive theory has given strong impetus to developing computational tools to solve the many-particle Schroedinger equation. I will review some of these theoretical highlights in nuclear structure, ranging from the modeling and computation of few-body systems to the many-particle finite systems represented by our heavy nuclei. Among the models I discuss are the unitary-limit fermionic Hamiltonian, the Nilsson model of nuclear deformations, and the Richardson-Gaudin model of pairing. Computational strategies that have been very successful in different contexts are the Monte-Carlo methods, the multi-configuration shell model, and the extensions of mean-field
theory to restore broken symmetries.

Presenter: BERTSCH, George

Contribution ID: **373** Type: **not specified**

Coffe break

Contribution ID: **374** Type: **not specified**

Round table

Monday, September 15, 2014 4:50 PM (40 minutes)

Contribution ID: **375** Type: **not specified**

Registration

Will be performed by Elizabeth Yang at her Office, Nordita main building, number 23.

Contribution ID: **376** Type: **not specified**

Registration

Monday, September 15, 2014 8:45 AM (45 minutes)

Performed by Nordita's secretary Elizabeth Yang. The registration will continue during the whole week. Therefore participants which do not reach to be registered during the period given here (i. e. 8:45 - 9:30) can do it afterwards, for instance within the lunch time.

Presenter: YANG, Elizabeth

Contribution ID: **377** Type: **not specified**

Boattrip with lunch

Saturday, September 20, 2014 12:00 PM (3 hours)

We take a boat through the many islands in the Stockholm Archipelago. The final destination is the beautiful village of Vaxholm, which is the only town in the inner Stockholm archipelago and therefore known as its capital. Lunch will be served during the trip.

Contribution ID: **378** Type: **not specified**

Discussion

Monday, September 15, 2014 12:20 PM (40 minutes)

Contribution ID: **379** Type: **not specified**

Time-Dependent Dynamics of Fermionic Superfluids: from cold atomic gases, to nuclei and neutron stars

Monday, September 15, 2014 11:00 AM (40 minutes)

The fascinating dynamics of superfluids, often referred to as quantum coherence revealed at macroscopic scale, has challenged both experimentalists and theorists for more than a century now, starting with electron superconductivity discovered in 1911 by Heike Kamerlingh Onnes. The phenomenological two-fluid model of Tizsa and its final formulation due to Landau, is ultimately a classical approach in which Planck's constant never appears and it is unable to describe the generation and dynamics of the quantized vortices, which are the hallmark characteristics of superfluidity. Various quantum mechanical phenomenological models have been developed over the years by London, Onsager, Feynman, Ginzburg and Landau, Abrikosov, and many others, but truly microscopic approaches are very scarce. The Gross-Pitaevskii equation was for many years the only example, but it is applicable only to a weakly interacting Bose gas at zero temperature and it has been used to describe the large variety of experiments in cold atomic Bose gases. In the case of fermionic superfluids only a time-dependent mean filed approach existed for a long time, which is known to be quite inaccurate. With the emergence of the Density Functional Theory and its time-dependent extension it became relatively recently possible to have a truly microscopic approach of their dynamics, which proves to be extremely relabel in predicting and describing various experimental results in cold atomic fermionic gases, nuclei and which can be used as well to make predictions about the nature and dynamics of vortices in the neutron star crust. I will describe the time-dependent superfluid local density approximation, which is an adiabatic extension of the density functional theory to superfluid Fermi systems and their real-time dynamics. This new theoretical framework has been used to describe/predict a range of phenomena in cold atomic gases and nuclear collective motion: excitation of the Higgs modes in strongly interacting Fermi superfluids, generation of quantized vortices, crossing and reconnection of vortices, excitation of the superflow at velocities above the critical velocity, excitation of quantum shock waves, domain walls and vortex rings in superfluid atomic clouds, and excitation of collective states in nuclei. This approach is the natural

framework to describe in a time-dependent framework various low energy nuclear reactions and in particular large amplitude collective motion and nuclear fission and the numerical implementation of this formalism requires the largest supercomputers available to science today.

Presenter: BULGAC, Aurel

Contribution ID: **380** Type: **not specified**

Lattice tight-binding Bogoliubov-de Gennes approach to nonuniform superconductivity: Josephson junctions, vortices, and disorder

I will present results on using a lattice tight-binding Bogoliubov-de Gennes formulation of nonuniform superconducting systems and solving self-consistently for the superconducting order parameter. Systems studied include Josephson junctions in graphene and spin-orbit coupled semiconductors, superconducting vortices in spin-orbit coupled semiconductors, and studies of the local effect of impurities and disordered edges in unconventional superconductors. While the method has limitations, especially with regards to system sizes possible to study, it offers a microscopically accurate description of the superconducting state, which can be crucial for a correct physical description of nonuniform superconducting systems.

Presenter: BLACK-SCHAFFER, Annica

Contribution ID: **381** Type: **not specified**

Lattice tight-binding Bogoliubov-de Gennes approach to nonuniform superconductivity: Josephson junctions, vortices, and disorder

I will present results on using a lattice tight-binding Bogoliubov-de Gennes formulation of nonuniform superconducting systems and solving self-consistently for the superconducting order parameter. Systems studied include Josephson junctions in graphene and spin-orbit coupled semiconductors, superconducting vortices in spin-orbit coupled semiconductors, and studies of the local effect of impurities and disordered edges in unconventional superconductors. While the method has limitations, especially with regards to system sizes possible to study, it offers a microscopically accurate description of the superconducting state, which can be crucial for a correct physical description of nonuniform superconducting systems.

Presenter: BLACK-SCHAFFER, Annica

Contribution ID: **382** Type: **not specified**

Neutrino physics and nuclear structure for double-beta decay

Neutrinoless double-beta decay, if observed, would signal physics beyond the Standard Model that would be discovered at energies significantly lower than those at which the relevant degrees of freedom can be excited. Therefore, it could be difficult to use the neutrinoless double-beta decay observations to distinguish between several beyond Standard Model competing mechanisms that were propose to explain this process. Accurate nuclear structure calculations of the nuclear matrix elements (NME) necessary to analyze the decay rates could be helpful to narrow down the list of competing mechanisms, and to better identify the more exotic properties of the neutrinos. In my talk I will review the neutrino physics relevant for double-beta decay, I will analyze the status of the shell model calculation of the NME, and their relevance for discriminating the contribution of possible competing mechanisms to the neutrinoless double-beta decay process. U.S. DoE grant DE-SC0008529 and U.S. NSF grants PHY-1068217 and PHY-1404442 are acknowledged.

Contribution ID: **383** Type: **not specified**

Angular-momentum-projection method to approach nuclear many-body wave functions

In performing shell-model calculations for large nuclear systems, the central issue is how to truncate the shell-model space efficiently. It corresponds to a proper arrangement of the configuration space to separate the most important part from the rest of the space. There are different schemes for the shell-model truncation. Considering the fact that most nuclei in the nuclear chart are deformed, using a deformed basis supplemented by angular momentum projection is an efficient way. Shell-model Hamiltonian is then diagonalized in the projected basis. The method is in principle independent of how a deformed basis is prepared and how an effective interaction is chosen. This approach may be viewed as to bridge the two traditional nuclear physics methods: the deformed mean-field approximation and the conventional shell-model diagonalization, because it keeps all the advantages that a mean-field model has to incorporate important correlations, and has the properties of the conventional shell-model that configurations are mixed beyond the mean-filed states to include effects of residual interactions. In this talk, we present the above idea by taking the Projected Shell Model and its extensions as examples [1,2,3,4]. Given the strong demand for shell model calculations also from nuclear astrophysics, one needs such an approach that contains sufficient correlations and can generate wave functions in the laboratory frame, thus allowing exact calculations for transition probabilities, spectroscopic factors, and beta-decay and electron-capture rates, in heavy, deformed nuclei. This research is supported by the National Natural Science Foundation of China (No. 11135005) and by the 973 Program of China (No. 2013CB834401). [1] K. Hara, Y. Sun, Int. J. Mod. Phys. E4 (1995) 637. [2] Y. Sun and C.-L. Wu, Phys. Rev. C68 (2003) 024315. [3] Y. Sun, Int. J. Mod. Phys. E15 (2006) 1695. [4] Y. Sun, Rev. Mex. Fis. S54(3) (2008) 122

Presenter: SUN, Yang

Contribution ID: **385** Type: **not specified**

Nuclear- and particle-physics aspects of condensed-matter nanosystems

The physics of condensed-matter nanosystems exhibits remarkable analogies with atomic nuclei. Examples are: Plasmons corresponding to Giant resonances [1], electronic shells, de- formed shapes, and fission [2], beta-type decay, strongly correlated phenomena associated with symmetry breaking and symmetry restoration [3], etc. Most recently, analogies with relativistic quantum-field theories (RQFT) and high-energy particle physics are beeing explored in the field of graphene nanostructures [4].
The talk will review these analogies focusing in particular on the following three aspects:
(1) The shell-correction method (SCM, commonly known as Strutinsky's averaging method and introduced in the 1960's in nuclear physics) was formulated [5] in the context of density functional theory (DFT). Applications of the DFT-SCM (and of a semiempirical variant, SE-SCM, closer to the nuclear Strutinsky approach) to condensed-matter finite systems will be discussed, including the charging and fragmentation of metal clusters, fullerenes, and metallic nanowires [5]. The DFT-SCM offers an improvement compared to the use of Thomas-Fermi gradient expansions for the kinetic energy density functional in the framework of orbital-free DFT.
(2) A unified description of strongly correlated phenomena in finite systems of repelling particles [whether electrons in quantum dots (QDs) or ultracold bosons in rotating traps] has been achieved through a two-step method of symmetry breaking at the unrestricted Hartree- Fock (UHF) level and of subsequent symmetry restoration via post Hartree-Fock projection techniques [3]. The general principles of the two-step method can be traced to nuclear theory (Peierls and Yoccoz) and quantum chemistry (L¨owdin). This method can describe a wide variety of novel strongly correlated phenomena, including:
(I) Chemical bonding and dissociation in quantum dot molecules and in single elliptic QDs, with potential technological applications to solid-state quantum computing.
(II) Particle localization at the vertices of concentric polygonal rings and formation of rotating (and other less symmetric) Wigner molecules in quantum dots and ultracold rotating bosonic clouds [6].
(III) At high magnetic field (electrons) or rapid rotation (neutral bosons), the method yields analytic trial wave functions in the lowest Landau level [7], which are an

alternative to the fractional-quantum-Hall-effect (FQHE) composite-fermion and Jastrow-Laughlin approaches.
(3) The physics of planar graphene nanorings with armchair edge terminations shows analo- gies with the physics described by the RQFT Jackiw-Rebbi model and the related Su-Schrieffer- Heeger model of polyacetylene [4]. This part of the talk will describe the emergence of exotic states and properties, like solitons, charge fractionization, and nontrivial topological insulators, in these graphene nanosystems.
[1] C. Yannouleas, R.A. Broglia, M. Brack, and P.F. Bortignon, Phys. Rev. Lett. 63, 255 (1989); [2] C. Yannouleas, U. Landman, and R.N. Barnett, in Metal Clusters, edited by
W. Ekardt (John-Wiley, New York, 1999) Ch. 4, p. 145; [3] C. Yannouleas and U. Landman, Rep. Prog. Phys. 70, 2067 (2007), and references therein; [4] I. Romanovsky, C. Yannouleas, and U. Landman, Phys. Rev. B 87, 165431 (2013); Phys. Rev. B 89, 035432 (2014). [5] C. Yannouleas and U. Landman, Phys. Rev. B 48, 8376 (1993); Ch. 7 in "Recent Advances in Orbital-Free Density Functional Theory," Y.A. Wang and T.A. Wesolowski Eds. (Word Scientific, Singapore, 2013) p. 203 (arXiv:1004.3536); [6] C. Yannouleas and U. Landman, Phys. Rev. Lett. 82, 5325
(1999); I. Romanovsky, C. Yannouleas, and U. Landman, Phys. Rev. Lett. 97, 090401 (2006). [7] C. Yannouleas and U. Landman, Phys. Rev. A 81, 023609 (2010); Phys. Rev. B 84, 165327 (2011).

Presenter: YANNOULEAS, Constantine

Contribution ID: **386** Type: **not specified**

Angular-momentum-projection method to approach nuclear many-body wave functions

Monday, September 15, 2014 3:10 PM (40 minutes)

In performing shell-model calculations for large nuclear systems, the central issue is how to truncate the shell-model space efficiently. It corresponds to a proper arrangement of the configuration space to separate the most important part from the rest of the space. There are different schemes for the shell-model truncation. Considering the fact that most nuclei in the nuclear chart are deformed, using a deformed basis supplemented by angular momentum projection is an efficient way. Shell-model Hamiltonian is then diagonalized in the projected basis. The method is in principle independent of how a deformed basis is prepared and how an effective interaction is chosen.
This approach may be viewed as to bridge the two traditional nuclear physics methods: the deformed mean-field approximation and the conventional shell-model diagonalization, because it keeps all the advantages that a mean-field model has to incorporate important correlations, and has the properties of the conventional shell-model that configurations are mixed beyond the mean-filed states to include effects of residual interactions.
In this talk, we present the above idea by taking the Projected Shell Model and its extensions as examples [1,2,3,4]. Given the strong demand for shell model calculations also from nuclear astrophysics, one needs such an approach that contains sufficient correlations and can generate wave functions in the laboratory frame, thus allowing exact calculations for transition probabilities, spectroscopic factors, and beta-decay and electron-capture rates, in heavy, deformed nuclei.
This research is supported by the National Natural Science Foundation of China (No. 11135005) and by the 973 Program of China (No. 2013CB834401).
[1] K. Hara, Y. Sun, Int. J. Mod. Phys. E4 (1995) 637.
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[3] Y. Sun, Int. J. Mod. Phys. E15 (2006) 1695.
[4] Y. Sun, Rev. Mex. Fis. S54(3) (2008) 122.

Presenter: SUN, Yang

Contribution ID: **387** Type: **not specified**

Neutrino physics and nuclear structure for double-beta decay

Wednesday, September 17, 2014 4:10 PM (40 minutes)

Neutrinoless double-beta decay, if observed, would signal physics beyond the Standard Model that would be discovered at energies significantly lower than those at which the relevant degrees of freedom can be excited. Therefore, it could be difficult to use the neutrinoless double-beta decay observations to distinguish between several beyond Standard Model competing mechanisms that were propose to explain this process. Accurate nuclear structure calculations of the nuclear matrix elements (NME) necessary to analyze the decay rates could be helpful to narrow down the list of competing mechanisms, and to better identify the more exotic properties of the neutrinos. In my talk I will review the neutrino physics relevant for double-beta decay, I will analyze the status of the shell model calculation of the NME, and their relevance for discriminating thecontribution of possible competing mechanisms to the neutrinoless double-beta decay process.
U.S. DoE grant DE-SC0008529 and U.S. NSF grants PHY-1068217 and PHY-1404442 are acknowledged.

Presenter: HOROI, Mihai

Contribution ID: **388** Type: **not specified**

Microscopic description of nuclear reactions within Coupled Cluster and Gamow Shell Model theories

Monday, September 15, 2014 4:10 PM (40 minutes)

Nuclei at drip-lines bear unique properties such as halos or resonant character at ground state level, inexistent in the valley of stability. While the latter consists of standard closed quantum systems, drip-line nuclei are open quantum systems, so that models describing their properties must include both nuclear inter-correlations and continuum degrees of freedom. Coupled Cluster and Gamow Shell Model theories, in both ab-initio and effective approaches, are tools of choice for that matter as nuclear correlations are present through configuration mixing while continuum degrees of freedom are imparted by the use of the Berggren basis. The latter methods, initially devised for structure calculations, can now be utilized to study reaction observables. Applications concern direct reactions on light and medium nuclei.

Presenter: MICHEL, Nicolas

Contribution ID: **389** Type: **not specified**

Lattice tight-binding Bogoliubov-de Gennes approach to nonuniform superconductivity: Josephson junctions, vortices, and disorder

Monday, September 15, 2014 11:40 AM (40 minutes)

I will present results on using a lattice tight-binding Bogoliubov-de Gennes formulation of nonuniform superconducting systems and solving self-consistently for the superconducting order parameter. Systems studied include Josephson junctions in graphene and spin-orbit coupled semiconductors, superconducting vortices in spin-orbit coupled semiconductors, and studies of the local effect of impurities and disordered edges in unconventional superconductors. While the method has limitations, especially with regards to system sizes possible to study, it offers a microscopically accurate description of the superconducting state, which can be crucial for a correct physical description of nonuniform superconducting systems.

Presenter: BLACK-SCHAFFER, Annica

Contribution ID: **390** Type: **not specified**

Nuclear- and particle-physics aspects of condensed-matter nanosystems

Monday, September 15, 2014 2:30 PM (40 minutes)

The physics of condensed-matter nanosystems exhibits remarkable analogies with atomic nuclei. Examples are: Plasmons corresponding to Giant resonances [1], electronic shells, de- formed shapes, and fission [2], beta-type decay, strongly correlated phenomena associated with symmetry breaking and symmetry restoration [3], etc. Most recently, analogies with relativistic quantum-field theories (RQFT) and high-energy particle physics are beeing explored in the field of graphene nanostructures [4]. The talk will review these analogies focusing in particular on the following three aspects:
(1) The shell-correction method (SCM, commonly known as Strutinsky's averaging method and introduced in the 1960's in nuclear physics) was formulated [5] in the context of density functional theory (DFT). Applications of the DFT-SCM (and of a semiempirical variant, SE-SCM, closer to the nuclear Strutinsky approach) to condensed-matter finite systems will be discussed, including the charging and fragmentation of metal clusters, fullerenes, and metallic nanowires [5]. The DFT-SCM offers an improvement compared to the use of Thomas-Fermi gradient expansions for the kinetic energy density functional in the framework of orbital-free DFT.
(2) A unified description of strongly correlated phenomena in finite systems of repelling particles [whether electrons in quantum dots (QDs) or ultracold bosons in rotating traps] has been achieved through a two-step method of symmetry breaking at the unrestricted Hartree- Fock (UHF) level and of subsequent symmetry restoration via post Hartree-Fock projection techniques [3]. The general principles of the two-step method can be traced to nuclear theory (Peierls and Yoccoz) and quantum chemistry (L¨owdin). This method can describe a wide variety of novel strongly correlated phenomena, including:
(I) Chemical bonding and dissociation in quantum dot molecules and in single elliptic QDs, with potential technological applications to solid-state quantum computing.
(II) Particle localization at the vertices of concentric polygonal rings and formation of rotating (and other less symmetric) Wigner molecules in quantum dots and ultracold rotating bosonic clouds [6].

(III) At high magnetic field (electrons) or rapid rotation (neutral bosons), the method yields analytic trial wave functions in the lowest Landau level [7], which are an alternative to the fractional-quantum-Hall-effect (FQHE) composite-fermion and Jastrow-Laughlin approaches.
(3) The physics of planar graphene nanorings with armchair edge terminations shows analo- gies with the physics described by the RQFT Jackiw-Rebbi model and the related Su-Schrieffer- Heeger model of polyacetylene [4]. This part of the talk will describe the emergence of exotic states and properties, like solitons, charge fractionization, and nontrivial topological insulators, in these graphene nanosystems.
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W. Ekardt (John-Wiley, New York, 1999) Ch. 4, p. 145; [3] C. Yannouleas and U. Landman, Rep. Prog. Phys. 70, 2067 (2007), and references therein; [4] I. Romanovsky, C. Yannouleas, and U. Landman, Phys. Rev. B 87, 165431 (2013); Phys. Rev. B 89, 035432 (2014). [5] C. Yannouleas and U. Landman, Phys. Rev. B 48, 8376 (1993); Ch. 7 in "Recent Advances in Orbital-Free Density Functional Theory," Y.A. Wang and T.A. Wesolowski Eds. (Word Scientific, Singapore, 2013) p. 203 (arXiv:1004.3536); [6] C. Yannouleas and U. Landman, Phys. Rev. Lett. 82, 5325 (1999); I. Romanovsky, C. Yannouleas, and U. Landman, Phys. Rev. Lett. 97, 090401 (2006). [7] C. Yannouleas and U. Landman, Phys. Rev. A 81, 023609 (2010); Phys. Rev. B 84, 165327 (2011).

Presenter: YANNOULEAS, Constantine

Contribution ID: **391** Type: **not specified**

Morning Session: BSC-BEC

Monday, September 22, 2014 9:45 AM (2 hours)

Temperature dependence of the pair coherence and healing lengths for a fermionic superfluid throughout the BCS-BEC crossover

The pair correlation function and the order parameter correlation function probe, respectively, the intra-pair and inter-pair correlations of a Fermi gas with attractive inter-particle interaction. Here, these correlation functions are
calculated in terms of a diagrammatic approach, as a function of coupling throughout the BCS-BEC crossover and of temperature, both in the superfluid and normal phase across the critical temperature T_c. Several physical quantities are obtained from this calculation, including the pair coherence and healing lengths, the Tan's contact, the crossover temperature T^* below which inter-pair correlations begin to build up in the normal phase, and the signature for the disappearance of the underlying Fermi surface which tends to survive in spite of pairing correlations. A connection is also established with experimental data on the temperature dependence of the normal coherence length as extracted from the proximity effect measured in high-temperature (cuprate) superconductors.

Presenter: CALVANESE-STRINATI, Giancarlo

Contribution ID: **392** Type: **not specified**

Afternoon Session: Metallic grains

Monday, September 22, 2014 2:30 PM (2 hours)

Chair: Alexander Balatsky

Presenter: ALHASSID, Yoram

Contribution ID: **393** Type: **not specified**

Morning Session: Density Functional Theories: Formalism and Applications

Tuesday, September 23, 2014 9:30 AM (2 hours)

Multi-Dimensionally Constrained Covariant Density Functional Theories: Formalism and Applications

Many different shape degrees of freedom play crucial roles in determining the nuclear ground state and saddle point properties and the fission path. For the study of nuclear potential energy surfaces, it is desirable to have microscopic and self-consistent models in which all known important shape degrees of freedom are included. By breaking both the axial and the spatial reflection symmetries simultaneously, we develop multi-dimensionally constrained covariant density
functional theories (MDC-CDFTs) [1-3]. The nuclear shape is assumed to be invariant under the reversion of x and y axes, i.e., the intrinsic symmetry group is V_4 and all shape degrees of freedom \beta_{\lambda\mu} with even \mu, such as \beta_{20}, \beta_{22}, \beta_{30}, \beta_{32}, \beta_{40}, …, are included self-consistently. The single-particle wave functions are expanded in an axially deformed harmonic oscillator (ADHO) basis. The functional can be one of the following four forms: the meson exchange or point-coupling nucleon interactions combined with the nonlinear or density-dependent couplings. The pairing effects are taken into account with either the BCS approach in MDC relativistic mean field (MDC-RMF) models [1,2] or the Bogoliubov transformation in MDC relativistic Hartree-Bogoliubov (MDC-RHB) models [3]. In this talk I will present the formalism of the MDC-CDFT's and the applications to the study of fission barriers and third minima in potential energy surfaces of actinide nuclei [1,2,4], the Y_{32} correlations in
N=150 isotones and Zr isotopes [5,6], and shape of hypernuclei [7,8].
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[3] B. N. Lu, et al., in preparation.
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[nucl-th].
[6] J. Zhao, et al., in preparation.
[7] B. N. Lu, E. G. Zhao, and S. G. Zhou, Phys. Rev. C84 (2011) 014328.
[8] B. N. Lu, E. Hiyama, H. Sagawa, and S. G. Zhou, Phys. Rev. C84 (2014) 044307.
Density Functional Theories: Formalism and Applications

Presenter: ZHOU, Shan-Gui

Contribution ID: **394** Type: **not specified**

Afternoon Session: Modern approaches to nuclear structure

Tuesday, September 23, 2014 2:30 PM (2 hours)

T. Suzuki

Nuclear shell structure, nuclear forces and nuclear weak processes

Shell-model study of spin modes in nuclei have been done with new shell-model Hamiltonians which have proper tensor components, and applied to nuclear weak processes at stellar environments. Roles of nuclear forces, especially the tensor and three-body interactions, on nuclear structure and shell evolutions are investigated. New shell-model Hamiltonians for p-shell (SFO [1]) and pf-shell (GXPF1[2]) and VMU (monopole-based universal interaction) [3], are found to describe spin-dependent modes in nuclei very well such as Gamow-Teller (GT) strength in 12C [1], 40Ar [4], 56Fe and 56Ni [5] and magnetic moments of p-shell nuclei [1,6], as well as shell evolutions toward drip-lines [3,7]. We discuss some of the following topics on nuclear weak processes at stellar environments with the use of the new transition strengths:
(1) New neutrino-nucleus reaction cross sections on light nuclei are used to study light-element nucleosynthesis in supernova explosions [8], and the production yield ratio for 11B/7LI is pointed out to be useful to determine the neutrino-mass hierarchy [9].
(2) New neutrino-induced cross sections are obtained for 13C [10] and 40Ar [4], which are useful targets for detection of solar and supernova neutrinos.
(3) New electron-capture rates in Ni isotopes [11] are obtained with GXPF1 and implications on element synthesis are studied.
(4) E-capture and beta-decay rates in sd-shell are used to study nuclear URCA processes in O-Ne-Mg core stars [12].
Roles of the three-body forces, especially the Fujita-Miyazawa force, on proper shell evolutions of neutron-rich isotopes [13], as well as on the closed-shell nature of 48Ca and M1 transition in 48Ca are also studied on top of the two-body G-matrix obtained by including core-polarization effects in larger spaces.

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2. M. Honma et al., Phys. Rev. C 65, 061301(R) (2002); 69, 034335 (2004).
3. T. Otsuka, T. Suzuki, H. Honma, Y. Utsuno, N. Tsunoda, K. Tsukiyama and M. Hjorth-Jensen, Phys. Rev. Lett. 104, 012501 (2010).
4. T. Suzuki and M. Honma, Phys. Rev. C 87, 014607 (2013).
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A. Idini
Nuclear Field Theory, Shell Model, Nuclear Reactions and Nuclear Astrophysics

Mean field, independent particles, picture is the starting point of our understanding of the nuclear many-body system. Many development across those lines in terms of treatment and effecting interaction, culminating in the last EDF efforts, enable us to study globally, across the whole nuclear chart, the bulk properties of nuclei. However including more complex nuclear correlations, is customary to exploit the
richness of nuclear structure in the related fields of nuclear reactions and astrophysics shedding light on specific, important cases and open problems like the origin of pairing in nuclei or the importance of forbidden decays in astrophysical processes. This can be achieved in terms of including correlation starting from a mean field, and then considering the interweaving of collective and single particle degrees of freedom (Nuclear Field Theory), which gives a reasonable estimate over several type of nuclear structure observables, remarking the dual origin of nuclear pairing
and enabling a quantitative account of direct nuclear reaction's absolute cross sections.
From another point of view, considering the contributions of the possible configurations, effectively interacting in a defined valence space (Shell Model), gives a precise estimate of ground and low-lying states. This is of outmost importance in
order to estimate quantities related to beta decay and electron capture, key in several astrophysical process, thus providing important insight to nuclear astrophysics.
* A. Idini et al., Dual Origin of Pairing in Nuclei,

http://arxiv.org/abs/1404.7365
* G. Potel et al., Cooper pair transfer in nuclei, RPP 76, 106301.
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* A. Idini et al., Quasiparticle renormalization and pairing correlations in spherical superfluid nuclei, PRC 85, 014331.
http://journals.aps.org/prc/abstract/10.110 /PhysRevC.85.014331

Presenters: IDINI, Andrea; SUZUKI, Toshio

Contribution ID: **395** Type: **not specified**

Morning session: Coupled Clusters

Wednesday, September 24, 2014 9:30 AM (2 hours)

Unconventional Coupled Cluster Theories for Strong and Weak Correlations

Coupled cluster (CC) theory with single and double excitations accurately describes weak electron correlation but is known to fail in cases of strong static correlation. Fascinatingly, however, pair coupled cluster doubles (p-CCD), a simplified version of the theory limited to pair excitations that preserve the seniority of the reference determinant (i.e., the number of unpaired electrons) has mean field computational cost and is an excellent approximation to the full configuration interaction (FCI) of the paired space provided that the orbital basis is optimized to adequately define a pairing scheme. In previous work [1], we have shown that optimization of the pairing scheme in the seniority zero FCI leads to a very accurate description of static correlation. The same conclusion extends to p-CCD [2] if the orbitals are optimized to make the p-CCD energy
stationary [3]. The extension of this pair model to quasiparticles will be addressed [4]. We additionally discuss renormalized Hamiltonians via similarity transformation based on Gutzwiller projectors and other exponential forms to describe residual weak correlations [5].
[1] Seniority and orbital symmetry as tools for establishing a full configuration interaction hierarchy, L. Bytautas, T. M. Henderson, C. A. Jimenez-Hoyos, J. K. Ellis, and G. E. Scuseria, J. Chem. Phys. 135, 044119 (2011).
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[5] Noncompact similarity transformed Hamiltonians for lattice models, J. Wahlen-Strothman, C. A. Jimenez-Hoyos, T. M. Henderson, and G. E. Scuseria, in preparation.

Presenter: SCUSERIA, Gustavo

Contribution ID: **396** Type: **not specified**

Afternoon Session: Coupled Cluster Methods

Wednesday, September 24, 2014 2:30 PM (2 hours)

SINGLE-REFERENCE COUPLED-CLUSTER METHODS FOR MULTI-REFERENCE MOLECULAR PROBLEMS

Piotr Piecuch, Jun Shen, Nicholas P. Bauman, and Jared A. Hansen

Accurate modeling of chemical reactions and photochemistry requires a balanced treatment of dynamical and non-dynamical many-electron correlation effects. The popular single-reference coupled-cluster (CC) and equation-of-motion CC (EOMCC) methods, such as CCSD(T) and EOMCCSD, capture the former effects very effectively, but have difficulties with the latter ones, whereas multi-reference CC theories that are supposed to capture both types of correlations continue facing unresolved problems. This talk will discuss pragmatic ways of addressing this situation via the completely renormalized and active-space CC and EOMCC theories, and their recent merger via the novel CC(P;Q) formalism, which reproduces the nearly exact relative and total electronic energies in ground and excited states at the small fractions of computer costs of other methods that aim at similar accuracies. The development of the singly and doubly ionized and electron-attached variants of the active-space EOMCC methodology, which provide an excellent description of electronic excitations in radicals, biradicals, and other similar open-shell systems around closed shells at the low computational costs compared to the parent approaches, will be addressed, too.

Presenter: PIECUCH, Piotr

Contribution ID: **397** Type: **not specified**

Morning Session: Variational Theories in Quantum Chemistry

Thursday, September 25, 2014 9:30 AM (2 hours)

Chair: Jorge Dukelsky

Presenter: AYERS, Paul

Contribution ID: **398** Type: **not specified**

Afternoon Session: Coupled Cluster Theories

Thursday, September 25, 2014 2:30 PM (2 hours)

Chair: Gustavo Scuseria

Presenter: DUGUET, Thomas

Contribution ID: **399** Type: **not specified**

(no title)

Chair: Osvaldo Civitarese

Presenters: ZHANG, Feng-Shou; REN, Zhongzhou

Contribution ID: **400** Type: **not specified**

Pairing Theory of the Wigner energy

Friday, September 26, 2014 2:30 PM (2 hours)

In 1936, Bethe and Bacher suggested that when the Coulomb energy is neglected, the masses of nuclei with given mass number A=N+Z, where N and Z are the numbers of neutrons and protons, rise from N=Z approximately quadratically in N-Z. Myers and Swiatecki found in 1966 a marked deviation from this rule; for small |N-Z| the mass rises more rapidly. They called the resulting apparent extra binding energy in the vicinity of N=Z the Wigner energy. It will be shown that this nonanalytic behaviour of the mass as a function of N-Z arises naturally when the pairing force is taken into account beyond a mean field approximation. In the limit of an equidistant single nucleon spectrum, the symmetry energy, that is, the increment of the mass from N=Z in the absence of the Coulomb energy, is proportional to T(T+1), where T is the isospin, in the ground state of a doubly even nucleus equal to |N-Z|/2. This expression is similar to the one which describes the spectrum of a quantal, axially symmetric rotor, and Frauendorf and Scheikh identified in 1999 the deformation which gives rise to an analogous rotation in isospace as the superfluid pair gap. Large shell corrections modify this bulk behaviour. In recent work by Bentley and Frauendorf, partly in collaboration with the speaker, various approaches to the treatment of these shell corrections are
considered. In one approach the pairing force is diagonalised exactly in a small valence space. More recently, the usual pairing correction of the Nilsson-Strutinsky theory is supplemented with a term derived from the Random Phase Approximation. The resulting theory reproduces quite well the empirical masses in the vicinity of N=Z for A not less
than 24. A very recent generalisation of the method, which allows its application throughout the chart of nuclides and also on top of a formalism of the Hartree-Fock type, will be discussed.

Presenter: NEERGAARD, Kai

Contribution ID: **403** Type: **not specified**

Morning Session: Dynamics of Quantum Open Systems

Monday, September 29, 2014 9:30 AM (2 hours)

Chair: Jonas Larson

Presenter: GUDMUNDSSON, Vidar

Contribution ID: **404** Type: **not specified**

Afternoon Session: Signature of the FFLO phase in the collective mode spectrum of ultracold Fermi gases

Monday, September 29, 2014 3:30 PM (1 hour)

We study theoretically the collective modes of a two-component Fermi gas with attractive interactions in a quasi-one-dimensional harmonic trap. We focus on an imbalanced gas in the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase. Using a mean-field theory, we study the response of the ground state to time-dependent potentials. For potentials with short wavelengths, we find dramatic signatures in the large-scale response of the gas which are characteristic of the FFLO phase. This response provides an effective way to detect the FFLO state in experiments.

Presenter: EDGE, Jonathan

Contribution ID: **405** Type: **not specified**

Morning Session: Alpha Condensates. Alpha-decay: a computational challenge

Tuesday, September 30, 2014 9:30 AM (2 hours)

Alpha-decay: a computational challenge
D.S. Delion, R.J. Liotta, and A. Dumitrescu
The microscopic description of alpha decay widths is an old but still challenging issue. The standard mean field plus residual interaction is not able to reproduce the absolute value of the decay width. We propose two ways to cure this defficiency, namely by introducing a new single particle diagonalization basis with two harmonic oscillator parameters [1] and by increasing proton-neutron correlations through a surface cluster component in addition to the standard nuclear the mean field [2]. We describe alpha decay fine structure by using a common approach for spherical, transitional and deformed nuclei [3]. The investigation of the alpha decay fine structure is a powerfull tool to probe nuclear structure. We use projected coherent states to describe the structure of daugher nuclei and a quadrupole-quadrupole alpha-core interaction for alpha transitions to excited states. It turns out that the strength of this interaction, reproducing alpha transitions to 2+ states, is proportional to the clustering probability. Predictions for electromagnetic and alpha transitions to excited state are made for all available even-even emitters. The coupled channel analysis for alpha transitions in odd mass nuclei is proposed as a promising tool to investigate nuclear structure, by the using both spectroscopic and alpha decay data.
This work was supported by the strategic grant POSDRU/159/1.5/S/137750 and by the grant PN-II-ID-PCE-2011-3-0092 of the Romanian ANCS.
[1] D.S. Delion, A. Insolia, R.J. Liotta, Physical Review C 54, 292 (1996).
[2] D.S. Delion, R.J. Liotta, Physical Review C 87, 024309 (2013).
[3] D.S. Delion, A. Dumitrescu, Physical Review C 87, 041302(R) (2013).

Presenters: DELION, Doru Sabin; SCHUCK, Peter

Contribution ID: **406** Type: **not specified**

Afternoon Session: Neutron-Nucleus Interactions at Low Energies

Tuesday, September 30, 2014 2:30 PM (2 hours)

Presenter: SUHONEN, Jouni

Contribution ID: **407** Type: **not specified**

Morning Session: Improving measurement precision with Weak Measurements

Wednesday, October 1, 2014 9:30 AM (2 hours)

The weak measurement protocol, introduced by Aharonov, Albert and Vaidman 25 years ago, is now in widespread use. They showed that weak coupling of a measurement device to a quantum system, together with a postselection, can yield an intriguing quantity which was named The Weak Value. In some contexts an observable on the system can be replaced by its Weak Value, even though it can be much larger than any of its eigenvalues and is also complex in general. The method of weak measurements have been shown to be highly useful both for the analysis of fundamental issues in quantum mechanics and for practical applications such as precision improvement. We will start with a review of the formalism and then discuss a recent development regarding the enhancement of the Signal to Noise Ratio for precision measurements in the presence of technical noise. We will see that when imaginary weak values are used, such a noise can improve the precision.
Reference: Y. Kedem, Phys. Rev. A 85, 060102 (R) (2012)

Presenter: KEDEM, Yaron

Contribution ID: **408** Type: **not specified**

Afternoon Session: Explosive Nucleosynthesis of heavy elements

Wednesday, October 1, 2014 2:30 PM (2 hours)

Presenter: MARTINEZ PINEDO, Gabriel

Contribution ID: **409** Type: **not specified**

Morning Session: Quantum Optics

Thursday, October 2, 2014 9:30 AM (2 hours)

Chair: Jorge Dukelsky

Presenter: LARSON, Jonas

Contribution ID: **411** Type: **not specified**

Morning Session: Approximate and exact Boltzmann machine learning for the US stock market

Friday, October 3, 2014 9:30 AM (2 hours)

Presenter: BORYSOV, Stanislav

Contribution ID: **412** Type: **not specified**

Afternoon Session: Mean field approaches

Friday, October 3, 2014 2:30 PM (2 hours)

Presenter: MENG, Jie

Contribution ID: **413** Type: **not specified**

Morning Session: Ab initio nuclear structure from lattice effective field theory

Monday, October 6, 2014 9:30 AM (2 hours)

I discuss recent results obtained using lattice effective field theory to probe nuclear structure. In particular I present recent lattice calculations of the Hoyle state of carbon-12 and whether or not light quark masses must be fine-tuned for the viability of carbon-based life.

Presenter: LEE, Dean

Contribution ID: **414** Type: **not specified**

Afternoon Session: Exotic nuclei. Bosonic embedded gaussian ensembles

Monday, October 6, 2014 2:30 PM (2 hours)

Jason Holt
Nuclear forces and exotic nuclei.

Within the context of valence-space Hamiltonians derived from different ab initio many-body methods, I will discuss the importance of 3N forces in understanding and making new discoveries in two of the most exciting regions of the nuclear chart: exotic oxygen and calcium isotopes. Beginning in oxygen, we find that the effects of 3N forces are decisive in explaining why 24O is the last bound oxygen isotope [1,2].
Furthermore, 3N forces play a key role in reproducing spectra, including signatures of doubly magic 22,24O, as well as properties of isotopes beyond the dripline. The calcium isotopes, with potentially three new magic numbers beyond the standard N=20,28, present a unique laboratory to study the evolution of shell structure in medium-mass nuclei. From the viewpoint of two-neutron separation energies and spectroscopic signatures of doubly-magic systems, I emphasize the impact of 3N forces in reproducing the N=28 magic number in 48Ca and in predicting properties of 50-56Ca, which indicate new N=32,34 magic numbers. Finally, I will highlight new efforts to quantify theoretical uncertainties in ab initio calculations of medium-mass nuclei by exploring resolution-scale dependence of observables in sd-shell isotopic/isotonic chains.

Adrian Ortega
Eigenvalue and eigenvector statistics for bosonic embedded gaussian ensembles

Within the framework in Random Matrix Theory (RMT), there exists the Bosonic Embedded Gaussian Ensembles. In the last few years, there has been a renewed interest in such ensembles. These ensembles display different eigenvalue and eigenvector correlations compared against the canonical ensembles of RMT. I shall describe briefly these bosonic ensembles when the single-particle states are two. Novel results will be presented for three single-particle states.
In this framework, I shall describe also some numerical experiments on a variation of the Bose-Hubbard model, namely the Random Bose-Hubbard model. Another ongoing interesting project is the study of quantum dynamics in disordered networks, and the roles that play the particle correlations that benefits the transition probability between two

ocupation-number states.

Presenters: ORTEGA, Hugo Adrian; HOLT, Jason

Contribution ID: **415** Type: **not specified**

Morning Session: Introduction to Monte Carlo simulations of neutrontransport in nuclear reactors. Development of new Monte Carlo methods for reactorphysics applications

Tuesday, October 7, 2014 9:30 AM (2 hours)

1)Introduction to Monte Carlo simulations of neutron transport in nuclear reactors

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2) Development of new Monte Carlo methods for reactor physics applications

Presenter: DUFEK, Jan

Contribution ID: **416** Type: **not specified**

Afternoon Session: On the entropy for quantum unstable states

Tuesday, October 7, 2014 2:30 PM (40 minutes)

We discuss some of the prescriptions available in the literature about the definition of thermodynamical observables for quantum unstable states. The formalism is based on the use of resonances (states with complex energies) in the path-integral formulation of path integrals and generating functions. The results are confronted mathematical oriented formulations of the problem.

Presenter: CIVITARESE, Osvaldo

Contribution ID: **417** Type: **not specified**

Morning Session: Strongly correlated electron systems

Wednesday, October 8, 2014 9:30 AM (2 hours)

Olivier Juillet
Intertwined orders in strongly correlated electron systems.

The quantum phase diagram of the two-dimensional Hubbard model is investigated through the mixing of unrestricted Hartree-Fock and BCS wave-functions with symmetry restoration before variation. The spin, charge, and superconducting orders entailed in such correlated states will be discussed as well as their evolution with hole doping and the on-site Coulomb repulsion. The relevance of the approach against exact results or numerical simulations when available will also be addressed.

Alexandre Leprévost
Exact ground state of strongly correlated electron systems from symmetry-restored wave-functions

The four site Hubbard model is considered from the exact diagonalization and variational method points of view. We show that a symmetry projected mean-field theory recovers the exact ground state energy, irrespective of the interaction strength, in contrast to the conventional Gutzwiller wave-function that will be also considered.

Presenters: LEPRÉVOST, Alexandre; JUILLET, Olivier

Contribution ID: **418** Type: **not specified**

Afternoon Session: Controlled healing of graphene nanopores

Wednesday, October 8, 2014 2:30 PM (2 hours)

Nanopores – nanometer-size channels hold significant promise for numerous applications: DNA sequencing, sensing, biosensing and molecular detectors, and catalysis and water desalination. However, these applications require accurate control over the size of the nanopores. Our simulations clearly point to at least two distinct healing mechanisms for graphene sheets: edge attachment (where carbons are attached to the edges of the graphene sheet/pore) and direct insertion (where individual atoms insert directly into a sheet of graphene, even in the absence of the edges). The insertion mechanism is a surprising prediction that points to the growth process that would be operational in pristine graphene. We have uncovered an unusual dependence in the speed of nanopore regrowth and the structure of ''healed'' areas as a function of its size in a wide range of temperatures. Our findings point to significantly more complicated pathways for graphene annealing.

Presenter: ZAKHARCHENKO, Kontantin

Contribution ID: **419** Type: **not specified**

Morning Session: Quantum computing

Thursday, October 9, 2014 9:30 AM (2 hours)

Hoshang Heydare
Introduction

Mohamed Bourennane
Quantum computing

Presenters: HEYDARI, Hoshang; BOURENNANE, Mohamed

Contribution ID: **420** Type: **not specified**

Afternoon Session: Hall viscosity of hierarchical quantum Hall states.

Thursday, October 9, 2014 2:30 PM (2 hours)

Using methods based on conformal field theory, we construct model wave functions on a torus with arbitrary flat metric for all chiral states in the abelian quantum Hall hierarchy. These functions have no variational parameters, and they transform under the modular group in the same way as the multicomponent generalizations of the Laughlin wave functions. Assuming the absence of Berry phases upon adiabatic variations of the modular parameter τ, we calculate the quantum Hall viscosity and find it to be in agreement with the formula, given by Read, which relates the viscosity to the average orbital spin of the electrons. For the filling factor $\nu = 2/5$ Jain state, which is at the second level in the hierarchy, we compare our model wave function with the numerically obtained ground state of the Coulomb interaction Hamiltonian in the lowest Landau level, and find very good agreement in a large region of the complex τ plane. For the same example, we also numerically compute the Hall viscosity and find good agreement with the analytical result for both the model wave function and the numerically obtained Coulomb wave function. We argue that this supports the notion of a generalized plasma analogy that would ensure that wave functions obtained using the conformal field theory methods do not acquire Berry phases upon adiabatic evolution.

Presenter: FREMLING, Mikael

Contribution ID: **421** Type: **not specified**

Morning Session: Quantum speed limits and optimal Hamiltonians for driven systems in mixed states

Friday, October 10, 2014 9:30 AM (2 hours)

Presenter: HEYDARI, Hoshang

Contribution ID: **422** Type: **not specified**

Afternoon Session: The Many-body localization transition

Friday, October 10, 2014 2:30 PM (2 hours)

Many-body localization is closely connected to some fundamental questions of quantum mechanics, like how and why quantum systems thermalize. It can protect quantum order at elevated temperatures and can potentially be important in the development of quantum memories. Many-body localization occurs in isolated quantum systems when Anderson localization persists in the presence of finite interactions. Despite strong evidence for the existence of a many-body localization transition a reliable extraction of the critical disorder strength has been difficult due to a large drift with system size in the studied quantities. In this talk I describe the challenges involved in this problem and explain our approaches, based on entanglement entropy, to understand it: (i) the variance of the half-chain entanglement entropy of exact eigenstates and (ii) the long time change in entanglement after a local quench from an exact eigenstate. With this we can estimate the critical disorder strength and its energy dependence. We investigate these quantities in a disordered quantum Ising chain that also has disorder protected quantum order at large disorder strength and provide evidence for it being a separate transition.

Presenter: KJÄLL, Jonas

Contribution ID: **423** Type: **not specified**

Welcome address

Monday, September 22, 2014 9:30 AM (15 minutes)

Alexander Balatsky is one of the four Professors at Nordita.
He is in Condensed Matter Physics.

Ramon Wyss is Professor at the Royal Institute of Technology
(KTH) and Vice President of International Affairs there.

Presenters: BALATSKY, Alexander; WYSS, Ramon

Contribution ID: **424** Type: **not specified**

Program Dinner

Tuesday, September 30, 2014 7:30 PM (3 hours)

Contribution ID: **425** Type: **not specified**

AlbaNova Colloquium: From Materials to Cosmology; Studying the Early Universe Under the Microscope

Thursday, October 2, 2014 3:00 PM (1 hour)

Presenter: SPALDIN, Nicola

Contribution ID: **426** Type: **not specified**

Computational challenges in modern nuclear physics

Friday, September 26, 2014 9:30 AM (2 hours)

Luis Robledo
Computational challenges in nuclear EDF calculations.

Zao-Chun Gao
Overlaps and matrix elements of physical operators between arbitrary HFB states.

Beyond mean field methods have been widely used in various many-body quantum systems. However, there still are some problems to be solved in the implementation of beyond mean field calculations. Especially for systems with large number of particles, such as heavy nuclei, the efficiency of beyond mean
field calculations becomes a very serious problem. Recently, we have tried to figure out a convenient way of calculating the overlap between arbitrary HFB vacua [1]. We also found some compact formulae for the matrix elements of physical operators (e.g. Hamiltonian) between arbitrary HFB multiquasiparticle states [2]. These formulae may reduce the computational time by several orders of magnitude when applied to many-body quantum system in a large Fock space.
[1] Zao-Chun Gao, Qing-Li Hu, Y. S. Chen Physics Letters B 732 (2014)360.
[2] Qing-Li Hu, Zao-Chun Gao, Y. S. Chen Physics Letters B 734 (2014)162.

Presenters: ROBLEDO, Luis; GAO, Zao-Chun

Contribution ID: **427** Type: **not specified**

Afternoon Session: Odd frequency pairing in hybrid structures and multiband superconductors

Monday, September 29, 2014 2:30 PM (40 minutes)

Odd frequency superconductivity proved to be an elusive state that is yet to be observed as a primary pairing state. On the other hand the list of systems and structures where odd frequency can be present as an induced component is growing. I will review various scenarios pointing to emergence of odd frequency pairing due to modifications of the primary conventional pairing. Recently we find that odd frequency component is ubiquitously present in multiband superconductors. We show that odd-frequency superconducting pairing requires only a finite band hybridization, or scattering, and non-identical intraband order parameters, of which only one band needs to be superconducting. From a symmetry analysis we establish a complete reciprocity between parity in band-index and frequency. I will also discuss extensions of the odd frequency superconductivity to the spin and boson systems.

Presenter: BALATSKY, Alexander

Contribution ID: **428** Type: **not specified**

Combined ab initio-mean field approach to solute-atom diffusion in alloys.

Tuesday, October 7, 2014 11:30 AM (40 minutes)

Solute diffusion in alloys is mostly mediated by defect-driven mechanisms. In irradiated materials, the considerably large point-defect population may enhance or even induce solute diffusion. In particular, in case of a binding solute-defect interaction, kinetic correlation effects may arise and lead to the formation of nanoscopic solute-defect complexes. The latter may be detrimental for the alloy structural integrity. In this talk we present a novel method for predicting the arising of solute-defect flux coupling in most types of alloys. The model combines first-principles calculations with an analytical mean field model and allows for the computation of solute transport and diffusion coefficients at low temperatures, which are usually inaccessible by means of experiments. The results for model dilute alloys will be presented, and implications on the structural integrity of nuclear reactor pressure vessel steels will be discussed.

Presenter: MESSINA, Luca

Contribution ID: **429** Type: **not specified**

Neutrino-nucleus scattering and supernova neutrinos

Tuesday, October 7, 2014 3:40 PM (40 minutes)

Neutrinos from core-collapse supernovae constitute valuable probes of both neutrino properties and of the currently unknown supernova mechanisms. Supernova neutrinos can be detected by using charged-current and/or neutral-current neutrino scatterings off nuclei. Theoretical estimates of the nuclear responses for relevant nuclei are important for the interpretation of future experimental results. The calculation of neutrino-nucleus cross sections constitute challenges both from the computational and theoretical points of view.
In this talk the challenges related to computations of neutrino cross sections will be discussed. Recent results of calculated nuclear responses for nuclei which are relevant for future neutrino experiments will also be presented.

Presenter: YDREFORS, Emanuel A.