2008 APS April Meeting and HEDP/HEDLA Meeting

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Saturday, April 12, 2008 10:45AM - 12:33PM –

Session B3 DNP GFB: Few Body Nuclear Physics I Hyatt Regency St. Louis Riverfront (formerly Adam039;s Mark Hotel), St. Louis E

10:45AM B3.00001 Auxiliary Field Diffusion Monte Carlo for nuclei and nuclear matter.[1] KEVIN SCHMIDT, Arizona State University — Quantum Monte Carlo methods have become a mainstream tool for understanding many-body quantum systems. The nuclear Hamiltonian with its strong spin-isospin dependence presents some special difficulties. I will describe the Auxiliary Field Diffusion Monte Carlo method which combines diffusion Monte Carlo sampling of the spatial positions of the nucleons along with an auxiliary field breakup that simplifies the sampling of the spin-isospin degrees of freedom. Results for nuclei, nuclear and neutron matter will be shown. The current state of the calculations, the approximations being made, and future prospects will be discussed.

[1]Supported by NSF Grant PHY-0456609

11:21AM B3.00002 Coupled-Cluster Theory for Molecular Structure and Spectra: The Challenges Posed By Molecules and the Coupled-Cluster Solutions[1] , RODNEY BARTLETT — Coupled-cluster (CC) theory derives from the ansatz that the n-particle wavefunction is $|\Psi$ >=exp(T)|0>, where T is an excitation operator with |0> some choice of mean-field wavefunction. That is sufficient to obtain energies. But to obtain anything else, we use the CC functional, E=<0|(!+Λ)exp(-T)Hexp(T)|0>, whose left and right hand eigenvectors provide energies and associated density matrices for the treatment of properties in CC theory. The introduction of Λ makes it possible to obtain the $\sim$3N forces associated with N atoms in the same time as the energy itself. This is essential information for indentifying the critical points on a potential energy surface and their associated Hessians, for either the prediction of vibrational spectra or to characterize a saddle point (transition state) for a reaction. A generalization of the functional to ω(k) =<0|L(k) exp(-T)Hexp(T)R(k)|0>, provides excitation energies, ω(k) along with excited state left- and right-hand wavefunctions, Finally, with the response functions obtained from these left- and right-hand eigenfunctions, used in closed form, higher-order properties like NMR coupling constants are obtained. In this way, coupled-cluster theory provides a method that addresses all the properties of interest for molecules and their interactions. This development will be the topic of our contribution. For details please see, R. J. Bartlett and M Musial, "Coupled-cluster theory in quantum chemistry", Revs. of Modern Phys. **79,** 291-352 (2007).

[1]This work was supported by U.S. Air Force Office of Scientific Research.

11:57AM B3.00003 Beyond the Shell Model: Computing Nuclei with Coupled-Cluster Theory , DAVID DEAN, Oak Ridge National Laboratory — Investigations of rare isotopes in the laboratory are opening the way to understand and clarify the properties of all nuclei and bulk nuclear matter. In this talk I will assess where we stand today in solving the nuclear problem and how future rare isotope facilities will impact our understanding of nuclei. The first part of the nuclear problem concerns our ability to describe complex nuclei using as input the basic interactions among protons and neutrons. Indeed, our community is on the verge of discovering how light nuclear systems are built from nuclear interactions that have their roots in QCD. I will describe this exciting frontier of research through illustrating recent progress in the nuclear implementation of coupled-cluster methods, a quantum many-body technique that enjoys great success in quantum chemistry. Nuclei offer some interesting challenges to coupled-cluster theory and quantum many-body theory generally: first, effective field theory implementations of the nuclear forces indicate the presence of a three-body force. Second, very weakly bound nuclei can best be described utilizing a single-particle basis consisting of bound and continuum states. In both cases, we have developed methods to solve for nuclear properties in these systems. I will also describe the computational requirements for the solution of the nuclear coupled-cluster problem. This research is supported by the U.S. Department of Energy under Contract Number DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory).

Saturday, April 12, 2008 1:30PM - 3:18PM –

Session D4 DNP GFB: Few Body Nuclear Physics II Hyatt Regency St. Louis Riverfront (formerly Adam039;s Mark Hotel), Promenade B

1:30PM D4.00001 The Three-Nucleon Analyzing Power Puzzle - The Past 20 Years[1] , WERNER TORNOW, Duke University & TUNL — The three-nucleon (3N) analyzing power $A_y(\theta)$ puzzle (3NAPP) refers to the failure of rigorous 3N calculations to account for the magnitude of the measured nucleon-deuteron $A_y(\theta)$ in the angular region of the A_y maximum (30% underprediction). The 3NAPP is a low-energy phenomenon and does not refer to $A_y(\theta)$ in the energy range above 100 MeV, where standard 3N forces contribute significantly to $A_y(\theta)$ in the angular region of the cross-section minimum. The 3NAPP was discovered by Witała, Glöckle and Cornelius in 1987 when they compared their rigorous 3N calculations to the neutron-deuteron (n-d) data of the Tübingen/TUNL group, although some evidence of a possible problem with describing $A_y(\theta)$ was already reported in 1986 by Koike and Haidenbauer. Before 1995 the 3NAPP was solely a n-d scattering phenomenon. However, with the Coulomb problem solved in 3N calculations by Kievsky, Viviani and Rosati in 1995 for energies below, and in 1999 for energies above the deuteron breakup threshold, the 3NAPP entered a new stage and included $A_y(\theta)$ in proton-deuteron (p-d) scattering as well as the vector analyzing power $iT_{11}(\theta)$ in d-p scattering. Although p-d phase-shift analyses and their comparison to theoretical phase shifts provided some insight into the physics of the 3NAPP, the accurate p-d data initially created a new problem at energies below about 5 MeV, until the theoretical treatment of the magnetic moment interaction by Witała et al. and Kievsky et al. provided a uniform picture. The recent inclusion of relativity in 3N calculations by Witała et al. has increased the 3NAPP at low energies considerably (by about 25% at 5 MeV). Furthermore, the new n-d $A_y(\theta)$ data obtained by Weisel et al. at TUNL confirmed our conjecture that the transition region between 20 MeV and about 35 MeV, above which the 3NAPP disappears, is poorly understood. Here, p-d data are needed to make progress. Currently, the hope is that the 3N force terms predicted by Chiral Effective Filed Theory in N3LO will eventually provide the correct explanation of the 3NAPP. However, the range of the required 3N force terms has to be about 3 fm in order to describe the $A_y(\theta)$ and $iT_{11}(\theta)$ data at $E_{c.m.}$=432 keV.

[1]Work supported by US DOE, Office of Nuclear Physics, Grant # DE-FG02-97ER41033

2:06PM D4.00002 Towards a Microscopic Density Functional Theory for Nuclei[1] , SCOTT BOGNER, Michigan State University — Density functional theory (DFT) has enjoyed spectacular success describing inhomogeneous many-electron systems in condensed matter physics and chemistry where *ab initio* methods become computationally prohibitive, as was recognized by the Nobel Prize awarded to Walter Kohn in 1998. Because of the computational limitations of *ab initio* methods in medium and heavy nuclei, DFT is the only tractable many-body method that can at present be applied across the entire table of nuclides. Remarkably simple phenomenological functionals of the Skyrme and Gogny type have enjoyed nearly four decades of impressive success describing a wide range of nuclear properties for many different mass regions. However, different parameterizations lead to uncontrolled (i.e., parameterization-dependent) extrapolations far from stability, with no reliable method to estimate the theoretical error bars. A primary objective of the SciDAC project "Building a Universal Nuclear Energy Density Functional (UNEDF)" is to develop a *microscopically-based*, energy density functional applicable to all nuclei in the form of a generalized Skyrme functional, with theoretical error bars for the different terms in the UNEDF to provide guidance for fine-tuning to data and to give controlled extrapolations away from stability. In this talk, I describe a promising route for achieving these objectives that combine recent advances in chiral effective field theory (EFT) inter-nucleon interactions, renormalization group (RG) techniques for nuclear systems, and nuclear many-body computational methods.

[1]Supported in part by Department of Energy Grant No. DE-FC02-07ER41457

2:42PM D4.00003 *Ab initio* no-core shell model with continuum[1] , PETR NAVRATIL, LLNL — The *ab initio* no-core shell model (NCSM) is a many-body approach to nuclear structure of light nuclei. The NCSM adopts an effective interaction theory to transform fundamental inter-nucleon interactions into effective interactions for a specified nucleus in a selected harmonic oscillator basis space [1]. The method is capable of predicting nuclear structure from inter-nucleon forces derived from quantum chromodynamics by means of chiral effective field theory [2]. NCSM extensions to the microscopic description of nuclear reactions are now under development. In my talk, I will first discuss our recent calculations of the ^{4}He total photo-absorption cross section using two- and three-nucleon interactions from chiral effective field theory [3]. I will then outline our effort to augment the NCSM by the resonating group method (RGM) technique to develop a new method capable of describing simultaneously both bound states and nuclear reactions on light nuclei [4]. This approach, which preserves translational symmetry and the Pauli principle, will allow us to calculate cross sections of reactions important for astrophysics and describe weakly-bound systems from first principles. I will present our first phase shift results for neutron scattering off ^{3}H, ^{4}He and ^{7}Li and proton scattering off ^{3}He, ^{4}He and ^{7}Be using realistic nucleon-nucleon potentials.

[1] P. Navrátil, J. P. Vary and B. R. Barrett, Phys. Rev. C **62**, 054311 (2000).
[2] P. Navrátil and V. G. Gueorguiev and J. P. Vary, W. E. Ormand and A. Nogga, Phys. Rev. Lett. **99**, 042501 (2007).
[3] S. Quaglioni and P. Navrátil, Phys. Lett. B **652**, 370 (2007).
[4] S. Quaglioni and P. Navrátil, arXiv:0712.0855.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344. Support from U.S. DOE/SC/NP (Work Proposal Number SCW0498) and the Department of Energy under Grant DE-FC02-07ER41457 is acknowledged.

Sunday, April 13, 2008 1:30PM - 3:18PM –

Session L14 GFB: Few-Body Systems Hyatt Regency St. Louis Riverfront (formerly Adam039;s Mark Hotel), St. Louis G

1:30PM L14.00001 Realistic NN Interactions in Momentum Space - Visual Comparisons[1] , A.G. NEGOITA, J.P. VARY, P. MARIS, Iowa State University, A. SHIROKOV, Moscow State University — It is challenging to gain physical intuition for non-local operators such as realistic NN interactions. In addition, whenever one truncates a local operator, such as approximating it in a finite matrix representation, one introduces non-locality. We portray contour plots in momentum space of the realistic NN interaction, JISP16 [1], as well as the identity operator and the kinetic energy operator truncated to a finite oscillator basis space. We present results as a function of the cutoff scale and compare with similar plots of the Chiral N3LO interaction [2] processed through the Similarity Renormalization Group (SRG) [3]. We visually search for well-matched features as a function of the renormalization scale as well as through the calculated nuclear properties resulting from these interactions [4]. A selection of these comparisons will be presented.
[1] A.M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber, Phys. Letts. B **644**, 33 (2007).
[2] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 04100R (2003).
[3] R. Furnstahl, www.physics.ohio-state.edu/∼ntg/srg/
[4] S. K. Bogner, R. J. Furnstahl, P. Maris, R. J. Perry, A. Schwenk, J. P. Vary, arXiv:0708.3754, Nuc. Phys. A (to appear).

[1]Supported in part by USDOE grants DE-FC02-07ER41457 and DE-FG-02-87ER40371.

1:42PM L14.00002 Measurement of the Cross Section and Analyzing Powers for $\vec{\mathrm{d}}$+p Elastic Scattering at 180 MeV[1] , C.D. BAILEY, E.J. STEPHENSON, A.D. BACHER, IUCF, A.M. MICHERDZINSKA, U. Winnipeg, J.G. MESSCHENDORP, A. BIEGUN, M. ESLAMI-KALANTARI, L. JOULAEIZADEH, N. KALANTAR-NAYESTANAKI, H. MARDANPOUR, H. MOEINI, A. RAMAZANI-MOGHADDAM-ARANI, S.V. SHENDE, H. WÖRTCHE, KVI, E. STEPHAN, U. Silesia, ST. KISTRYN, Jagiellonian U., K. SEKIGUCHI, RIKEN — We have measured cross sections and analyzing powers for various $\vec{\mathrm{d}}$+d reaction channels, including $\vec{\mathrm{d}}$+d elastic and $\vec{\mathrm{d}}$+d→p+t at 130 MeV and 180 MeV, with the hope of providing a testing ground for new 4-body theoretical predictions. These data were collected at the KVI cyclotron (Groningen) using the Big Bite spectrometer and a polarized deuteron beam. In addition to the $\vec{\mathrm{d}}$+d channels, we also measured the cross section and analyzing powers (A_y and A_{yy}) for $\vec{\mathrm{d}}$+p elastic scattering at the same energies for comparison with existing data and with 3-body calculations (with and without three nucleon forces). We report here our results for the $\vec{\mathrm{d}}$+p elastic data at 180 MeV. The analysis procedure will be reviewed and several preliminary results will be shown.

[1]Work supported in part by NSF grant PHY-0457219

1:54PM L14.00003 Cluster separability and currents in the Poincaré invarant three-nucleon problem[1] , MARK TUCKER, University of Iowa, BRADLEY KEISTER, NSF, WAYNE POLYZOU, University of Iowa — We examine the quantitative implication of the requirement of cluster separability in Poincaré-invariant formulations of the quantum mechanical three-body problem. One can formulate the problem using two-body interactions in a representation that satisfies Poincaré invariance, but which violates cluster separability. An additional non-trivial unitary transformation restores cluster properties. This unitary transformation is needed for a consistent computation of matrix elements of currents that have cluster expansions in systems of three particles or more, as well as bound-state properties of four particles or more. We exhibit the nature and size of these effects in a model form factor of a three-body system consisting of a nucleon in the presence of a spectator deuteron by comparing the calculation of current matrix elements with and without these unitary transformations.

[1]This work supported in part by U.S. D.O.E. contract No. DE-FG02-86ER40286

2:06PM L14.00004 A realistic three-nucleon interaction in the ^{4}He scattering system[1] , JOHANNES KIRSCHER, HARALD GRIESSHAMMER[2], The George Washington University — Using the framework of the refined resonating group (RRGM) variational technique we investigate the $J^\pi = 0^+$ partial wave of the ^{4}He scattering system for an adjusted version of the realistic Illinois potential model (IL) which was devised as an extension of the Urbana IX (UIX) model. We compare the results to an R-matrix analysis and an RRGM calculation for the UIX potential. The binding energy, the S-, P-, D-state probabilities, the average charge- and mass radii of the ^{4}He bound state are given as well. We find all results consistent with the UIX ones and note only a difference in the t-p and ^{3}He-n phase shifts in the region of the $T = 0$ resonance.

[1]The grant of computing time at the RRZE is gratefully acknowledged.
[2]first author's thesis adviser

2:18PM L14.00005 ABSTRACT WITHDRAWN —

2:30PM L14.00006 ABSTRACT WITHDRAWN —

2:42PM L14.00007 Theoretical Fully Differential Cross Sections for Four-Body Processes , A.L. HARRIS, J.L. PEACHER, M. SCHULZ, D.H. MADISON, Missouri University of Science and Technology — Atomic collisions present a valuable opportunity to study the few body problem. Advances on the theoretical side now allow for an essentially exact numerical calculation of one of the simplest the few-body problems - the three-body problem. However, study of the four-body problem is still in its infancy, and the agreement between experiment and theory for kinematically complete experiments is far from satisfactory. The simplest four-body problem is a charged particle collision with helium in which both atomic electrons change state. Two theoretical models will be discussed for several possible outcomes of this type of collision. The first Born approximation (FBA) treats the projectile as a plane wave, and ignores the post collision Coulomb interaction between the two final state continuum electrons. The more sophisticated four-body distorted wave (4DW) model treats all continuum particles as distorted waves and explicitly includes the post collision Coulomb interaction between the two outgoing electrons. Fully differential cross sections calculated using the FBA and 4DW models will be compared to absolute experimental results, as well as other theories.

2:54PM L14.00008 Solving Schrodinger Equation in Mixed Representation , MALLIKA DHAR, CHARLES WERNETH, The University of Southern Mississippi, CHRISTOPHER SIROLA, KHIN MAUNG, The University of Southern Mississippi, USM COLLABORATION — Solving the Schrodinger equation with relativistic kinematics is easier in momentum space since the momentum operators under the radical sign simply become numbers. But power law potentials become singular in momentum space and subtraction procedures become necessary. By using the coordinate representation for the potential part and momentum representation for the kinetic energy part, one can solve these problems, but the resulting equation has an oscillating integral with a spherical Bessel function. We expand the wave function in a complete set of basis functions which has an exact Fourier transform and study the convergence of the solution by using different integration methods.

3:06PM L14.00009 Physical Properties of Human Whole Salivary Mucin:A Dynamic Light Scattering Study , MANISH MAHAJAN, All India Institute of Medical Sciences, New Delhi, VIJAY KUMAR, MAYANK SARASWAT, SAVITA YADAV, N.K. SHUKLA, T.P. SINGH, DR. BHIM RAO AMBEDHKAR INSTITUTE OF ROTARY CANCER HOSPITAL COLLABORATION — Human salivary mucin, a primary mucous membrane coating glycoprotein forms the first line of defense against adverse environments, attributed to the complex formation between mucin subunits and non mucin species. Aim of the study was to emphasize the effect of pH, denaturants (guanidinum hydrochloride, urea) and detergents (CHAPS, TRITON X -100, SDS on human whole salivary mucin. Hydrodynamic size distribution was measured using DLS. It was observed that aggregation was due to increase in hydrophobic interactions, believed to be accomplished by unfolding of the protein core. Whereas, the detergents which solubilize the proteins by decreasing hydrophobicity lead to disaggregation of mucin into smaller fragments. Mucin subjected to tobacco extract and upon subsequent addition of nicotine was found to have a disaggregating effect on it, suggesting nicotine may be one of the factors responsible for the disaggregating effect of tobacco on mucin, an important carcinogenetic mechanism.