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GAUSTEQ report on research conducted as well as discussions and planning sessions with collaborators in Germany during visit July 1 – August 18, 2012

Summary (see details blow)
During this to Germany, US and German collaborators succeeded in moving aggressively forward on two major multi-institution research projects: (A) Evaluating nuclear spectra and observables of light nuclei with chiral NN + NNN interactions; (B) incorporating chiral 1-body and 2-body current corrections to electroweak observables in light nuclei.

Itinerary:

July 1	depart from the US (Des Moines airport)
July 2-4	visit Technishe Universitaet Darmstadt
July 5-7	visit University of Bochum & deliver seminar (no GAUSTEQ support requested for this trip or period of time)
July 8-13	invited talk at Light Cone 2012 conference in Krakow, Poland (no GAUSTEQ support requested for this trip or period of time) (Note: J. Wambach, F. Lenz, N. Stefanis, C. Weiss also attended)
July 14-21	visit Technishe Universitaet Darmstadt
July 22-24	attend Computational Nuclear Physics Town Meeting – Washington, DC (no GAUSTEQ support requested for this trip or period of time)
July 25-29	visit Technishe Universitaet Darmstadt
July 30-Aug 3	invited talk at Argonne Theory Institute (no GAUSTEQ support requested for this trip or period of time) (Note: R. Roth, E. Epelbaum also attended)
Aug 4-18	visit Technishe Universitaet Darmstadt and one day at GSI (Aug. 14), returning to Des Moines on August 18.

The dates (inclusive of initial travel to Germany and final departure from Germany) that are associated with the GAUSTEQ award are: July 1-4, July 14-21, July 25-29 and Aug. 4-18. These dates correspond to 4 + 8 + 5 + 15 = 32 total days of GAUSTEQ-related activity. However, It is ok with me to cap the GAUSTEQ expenses at 31 days since that is what I had in the original proposal – simply correct the amounts accordingly in the expense summary.

<u>Chronology of physics research and meetings/discussions/planning activities during trip</u>

July 1: 8:45am – depart from home in West Des Moines, Iowa, for Des Moines airport
10:58am - depart Iowa on United flight to Chicago

July 2: 10:00am - arrive Frankfurt on United flight from London
meet with Prof. Robert Roth's group 1pm – 4pm initial planning sessions

July 3: meet with Prof. Robert Roth's group for initial discussions on 7Li and 8Li calculations with chiral NN + NNN interactions. Flesh out the planning document for the benchmark 12C project. Begin preparing tables of results as a function of basis space parameters and Similarity Renormalization Group (SRG) scale.

July 4: Higgs discovery by LHC announced in the morning so there was considerable discussion of this discovery with many members of the Nuclear Theory Institute
Then, met with Prof. Robert Roth's group for:

(1) Detailed comparison of 7Li and 8Li results with chiral NN + NNN interactions. We focused on the similarities and differences of spectra and electromagnetic moments and transition rates obtained in the largest basis spaces currently available (Nmax = 8) between the Okubo-Lee-Suzuki (OLS) renormalization scheme and the Similarity Renormalization Group (SRG) method. The OLS results were obtained using the Iowa State code Many Fermion Dynamics-nuclear (MFDn) and the SRG results were obtained using the Darmstadt Importance Truncated – No Core Shell Model (IT-NCSM) code. The results from an initial sample of observables turned out to be surprisingly consistent with each other so it was decided to expand the list of observables to explore more completely the range of similarities and differences. Preliminary results with Nmax = 10 from the IT-NCSM results were also examined to investigate the dependence on Nmax truncation. Reasonable convergence was found (few percent changes in going from Nmax = 8 to 10) when the SRG renormalization scale was set at $\lambda = 1.88$ fm^{-1}.

(2) study on scaling performance results for MFDn running on Jaguar at Oak Ridge National Lab and the IT-NCSM code running on Hopper at the National Energy Research Supercomputer Center (NERSC) at Lawrence Berkeley National Lab (LBNL). Initial scaling study of the IT-NCSM code showed good scaling on a test problem running on 2000 to 8000 cores. Further timing studies of this test case will now be obtained at 10,000 cores. Then a larger test case will be selected for scaling tests on 10,000 to 70,000 cores. Results for these runs will be obtained and reviewed in the coming weeks. The goal is to improve the IT-NCSM code to achieve leadership-class scaling performance (good scaling at and above 60,000 cores) so the IT-NCSM code may become a component of future INCITE applications in collaboration with the current INCITE award group (J. Vary is the PI of the current 3-year award which will lead to a new proposal in 2013).

(3) discussion of future plans for larger scale runs of MFDn and IT-NCSM with ambitious physics goals. We discussed plans for Nmax = 12 runs for all p-shell nuclei using chiral NN + NNN interactions. Physics goals include a first look at states in the p-shell which are expected to exhibit either strong NNN interaction effects or significant clustering effects or both. The disruptive technology of NVIDIA accelerators incorporated into Titan at ORNL became a major focal point of the discussions. How to work within the constraints of IO and memory limits of the accelerator pose a major problem that will require extensive investigation and some breakthrough ideas. We discussed some initial thoughts on partitioning the large NNN interaction files and coding for multiple passes through the partitions for constructing the many-body Hamiltonian.

July 4: 4:40 pm depart by train for Bochum and arrive at 8:08pm – met by Prof. Evgeny Epelbaum and driven to hotel.

July 5-6: Meet with Prof. Epelbaum's group (Hermann Krebs, students) to discuss plans for using their developing chiral NNN interactions, complete through N3LO, in nuclear many-body calculations. The extension of their efforts to obtain the higher partial wave decompositions of the complete NNN interactions at N3LO will involve efforts

currently underway at Ohio State University (Prof. Richard Furnstahl and post doc Dr. Kai Hebeler).

It became clear that further meetings and discussions would be needed to solidify plans for a wide-ranging set of international collaborations involving multiple institutions (Bochum, Juelich, Cracow, Darmstadt, Ohio State, Iowa State, TRIUMF). We scheduled a follow-up meeting with Prof. Evgeny Epelbaum, Prof. Robert Roth, Prof. Richard Furnstahl and Dr. Petr Navratil at the Argonne Theory Institute July 29 – Aug 3 which all of us will attend.

July 7-13: Travel to/from Cracow to participate in LC2012 (funding from other sources)

July 13: Met with Dr. Roman Skibinski in Cracow to discuss calculations of the partial wave decomposition of the newest three-nucleon forces (3NFs) that are complete through N3LO. This work, which is critical to our planned applications in light nuclei, may proceed to completion much more rapidly if the Cracow group would gain access to significant computational resources such as those envisioned in the INCITE program. We made a plan to propose a multi-institution collaboration to carry out the partial wave decompositions in two ways – one with anti-symmetrization "on one side" (useful for applications with Faddeev and Faddeev-Jacobovsky equations) and "on both sides" (useful for applications in light nuclei with ab initio no-core methods). Dr. Skibinski agreed to write an email to all concerned proposing the multi-institution collaboration and he did so on the same day (in outline form). He will provide a more detailed plan, including details on the scalability of the codes, run time estimates, etc., when he returns from vacation in mid-August.

July 14: Return to Darmstadt; research on light nuclei, read recent papers on the arxiv

July 15-21 and July 25-29:

(1) Met frequently with Prof. Robert Roth and his group (joined by Prof. Pieter Maris on July 18 and following days). Together, we planned tests of scaling performance of the IT-NCSM code, implementation of GPU strategies for decoupling the 3NFs, and completion of next-generation 3NFs in a partial wave decomposition. We made additional plans for the discussions at the Argonne Theory Institute. We decided that one of Prof. Roth's graduate students, Angelo Calci, should become a collaborating team member on Repo m94 at NERSC and begin some of the collaborative calculations there (I am the PI on this NERSC award of supercomputer resources). We therefore took the required steps to get him an account on m94 at NERSC. We refined our plans for the joint project, "Ab initio calculations of 12C with chiral NN+NNN interactions," to specify where we would carry out detailed calculations for uncertainty quantifications. We expanded the list of hbar-omega values since we have found that larger values provide results that are more stable with respect to the UV cutoff in the SRG evolution. We also added an NN-only case to the benchmarks as this is the largest component of the interactions and we are interested in the results for the rms radius for this case.

(2) Met a number of times with Dr. Javier Menendez to discuss the status of our 14C beta decay project in collaboration with Prof. Achim Schwenk and Prof. Doran Gazit. This project aims to evaluate the corrections to the Gamow-Teller decay arising from 1-body and 2-body currents according to chiral effective field theory (EFT). Since this decay is strongly suppressed by the contributions of chiral 3NFs, we expect significant corrections from chiral EFT. The Iowa State group has provided the one-

body density matrices for this collaborative project from the structure calculations reported in our paper (P. Maris, J. P. Vary, P. Navratil, W.E. Ormand, H. Nam, D. J. Dean, "Origin of the anomalous long lifetime of 14C," Phys. Rev. Lett. 106, 202502(2011). We reviewed the status of the present approximate calculations of the corrections from 1-body and 2-body currents. We prepared for more extensive discussions with Prof. Achim Schwenk when he returns to Darmstadt. At that time, we will decide whether full 2-body current evaluations are needed – i.e. where we do not make an average over one of the nucleons.

Aug. 6:

(1) Met with Prof. Robert Roth's students and discussed progress in achieving the partial wave decomposition of the 3NFs from Bochum. There is a current disagreement in results obtained from two different codes and there is a suspicion of a lack of precision in the numerical integration procedures of one of the codes. This will be checked by increasing the number of grid points which is challenging since the calculational effort increases as the fifth power of the number of grid points.
(2) Met with Prof. Achim Schwenk for an initial discussion of plans for the next couple of weeks. We began a review of the current status of our calculations on the 1-body and 2-body current corrections to the GT matrix element in 14C and we will continue this discussion throughout the week.

Aug 7 – 13:

Meetings with Prof. Achim Schwenk and his group to discuss a longer term large project where chiral two-body current corrections are routinely evaluated for electroweak processes that are obtained within the ab initio NCSM. This project will necessarily involve setting up a large scale collaboration involving Prof. Doran Gazit and a team of ab initio NCSM researchers committed to evaluating and storing two-body density matrices. We had one conference call with Prof. Gazit who is strongly supportive and suggested an initial target application - the beta decay from the ground state (GS) of 16N (2- state) to the GS of 16O (0+ state). This case should show minimal corrections arising from the chiral two-body currents and the quality of the agreement with experiment will be a direct test of the wavefunctions for this problem. Action agenda for JPV: Explore with Prof. Pieter Maris the plans for evaluating the two-body density matrices – should this be a stand-alone code (external to MFDn) or an internal option? Probably both are desired but for different applications. The stand-alone would be needed for the 16N -> 16O beta decay project, for example. We should discuss the stand-alone code with the student of Prof. Christian Forssen who should come to Ames in September for an extended visit. JPV will also assess the feasibility of an Nmax =8 calculation of the 16N spectroscopy – the dimensions ~ 3 billion, I estimate. A follow-up conference call was scheduled for Thursday, August 16, at 1:00pm.

Aug. 14:

Met with Dr. Thomas Neff at GSI to discuss:

a) clustering in light nuclei
b) two-nucleon correlations and two-nucleon density matrices
c) JISP16 NN interaction – approximated in operator form

Brief overview of those discussions

a) clustering in light nuclei – follow up to our discussions at HITES-2012 in New Orleans where he has now decomposed results of his cluster model calculations for 12C into the HO basis using a range of HO frequencies. I orgininally raised this question since he has previously presented this decomposition at a single frequency (20 MeV) which means that it may produce a pessimistic prediction that a rather high Nmax value may be needed (~40) to reproduce the Hoyle state clustering he obtains in his cluster-model results using the Volkov interaction. Indeed, he showed me results for as low as a HO frequency as 8 MeV where the required basis was still decreasing in Nmax. This led to the speculation that it may be that a HO frequency of 5 MeV may be optimal – i.e. where the required Nmax is as low as ~24 to obtain a good description. This result would be encouraging to the collaborative efforts with the LSU group (Draayer, Dytrych, et al) to develop the symmetry-adapted shell model with capabilities to evaluate 12C up to Nmax = 24 .
b) two-nucleon correlations and two-nucleon density matrices – Dr. Neff uses the two-nucleon correlation function (as a function of relative distance with the two-nucleon cm – momentum fixed at zero) to search for evidence of clustering. For example, the two-nucleon correlation function for the Hoyle state, minus 3 times the alpha particle two-nucleon correlation function exhibits a clear long-range character with all short-range components removed. This is another strong motivation for the Iowa State group to press forward to develop the capability to evaluate two-nucleon density matrices within MFDn along with the current option to evaluate the one-body density matrices.
c) JISP16 NN interaction – approximated in operator form
Dr. Neff showed me the results on his MS student's work to carry out the fit of JISP16 matrix elements in momentum space to an operator-form using conventional NN scattering potential operators. The radial forms are taken to be a sum of Gaussians with coefficients determined by fitting. The results obtained so far are encouraging up through partial waves with J = 2 (and below) but deteriorate for J = 3 and become unacceptable (judging from the comparison of phase shifts) for J = 4 partial waves. After some study and discussion we arrived at the conclusion that the L^2 term is probably leading to pathology in the higher partial waves – e.g. the spoiling of the desired OPEP behavior as one increases L. This suggests an improved approach where the L^2 operator is restricted to have only short distance coordinate-space functions multiplying it. Dr. Neff will see if the student can adjust his fitting process to achieve an improved fit.