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Abstract: The Junior Investigator grant “Structure of Rare Isotopes” (DE-FG02-07ER41529) supported research in low-energy nuclear theory from September 1, 2007 to August 31, 2010. It was the main goal of the proposed research to develop and optimize an occupation-number-based energy functional for the computation of nuclear masses, and this aim has been reached. Furthermore, progress was made in linking two- and three-body forces from low-momentum interactions to pairing properties in nuclear density functionals, and in the description of deformed nuclei within an effective theory.

Final Report

Mass formulae, i.e. parameterizations of nuclear binding energies as a function of neutron and proton numbers, are very accurate tools for the computation of nuclear masses. While the formulae are computationally very efficient, it is difficult to judge their predictive power in extrapolations into unknown regions of the nuclear chart, and they are difficult to improve. From a theoretical point of view, binding energies of atomic nuclei must result from a Hamiltonian or energy functional, and such an approach can allow theorists to seek systematical improvements and to compute other bulk properties (such as radii, deformations) besides the energy.

This grant funded the development of an occupation-number-based energy functional that is based on the theorems by Hohenberg and Kohn and takes shell-model occupations as the relevant degrees of freedom. For simple systems such as the Lipkin model, such a functional can be constructed explicitly via a Legendre transformation of the ground-state energy with respect to single-particle energies. The resulting functional is non-analytical in the differences of occupation numbers, and the minimization of the functional with respect to the occupation numbers yields the ground-state energy and ground-state occupations, see Publication #1. For the description of nuclei across the nuclear chart, the investigators employed a functional with phenomenological terms (motivated by the Duflo-Zuker mass formula) and analytical insights from their study of the Lipkin model. Guiding principles employed in the construction of suitable terms were saturation (i.e. correct scaling with mass number), and an efficient mechanism was developed to test candidate terms that might enter the functional. The resulting 17-parameter functional for nuclear binding energies was optimized to about 2000 nuclei of the nuclear chart, and a root-mean-square deviation of about 1.3 MeV was achieved. Extrapolation properties and stability of the functional was checked in optimization to a smaller number of nuclei. For details, see Publication #8.

Bulk nuclear properties are traditionally described with energy-density functional theory. Here, the main problem consists of linking the energy functional to the underlying Hamiltonian. One promising approach is based on low-momentum Hamiltonians that employ two- and three-nucleon interactions and result from realistic interactions (e.g. interactions from chiral effective field theory) after renormalization group transformations. Low-momentum Hamiltonians are amenable to perturbative calculations, and mean-field calculations can be used as in leading order. This establishes the link to density functional theory. Within such an approach the investigators describe pairing properties of finite nuclei and nuclear matter in a non-empirical manner, see Publications #2-6, 9.

Nuclear deformation is an emergent phenomenon, and the corresponding collective excitations introduce a very small energy scale (40 keV in actinides and 80 keV in rare earth nuclei) that separates from higher-energetic vibrations (of order 1 MeV). While deformed nuclei are traditionally understood in terms of geometric collective models and/or algebraic models, one can exploit the separation of scale and develop a systematic and model-independent description within the framework of an effective theory, see Publication #7.

Personnel

This grant partially supported the research of Bertolli during his PhD thesis (Bertolli graduated in 2011), the work of Postdoctoral Researcher Lesinski, and the research of the PI.

Publications and Talks

<u>PI / investigator</u>	<u>Publ.</u>	<u>prept./sub.</u>	<u>conf. rpts.</u>	<u>Talks</u>
Papenbrock	3	0	0	6
Lesinski	7	0	0	6
Bertolli	2	0	0	5
Total	10	0	0	17

Efforts not reported in this grant yielded another 12 referred journal publications and 10 invited presentations for the PI during 9/2007-8/2010. The list of journal publications below includes research that was initiated during the funding period but published after the completion of the funding period.

Journal Publications

1. *Energy functional of the three-level Lipkin model*, M. G. Bertolli and T. Papenbrock, Phys. Rev. C **80**, 064310 (2008).
2. *Non-empirical pairing energy density functional. First order in the nuclear plus Coulomb two-body interaction*, T. Lesinski, T. Duguet, K. Bennaceur and J. Meyer, Eur. Phys. J. A **40**, 121 (2009).
3. *Non-empirical pairing energy functional in nuclear matter and finite nuclei*, K. Hebeler, T. Duguet, T. Lesinski and A. Schwenk, Phys. Rev. C **80**, 044321 (2009).
4. *Tensor part of the Skyrme energy density functional II: Deformation properties of magic and semi-magic nuclei*, M. Bender, K. Bennaceur, T. Duguet, P.-H. Heenen, T. Lesinski and J. Meyer, Phys. Rev. C **80**, 064302 (2009).
5. *Instabilities in the nuclear energy density functional*, M. Kortelainen and T. Lesinski, J. Phys. G **37**, 064039 (2010).
6. *Nuclear Energy Density Optimization*, M. Kortelainen, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild, Phys. Rev. C **82**, 024313 (2010).
7. *Effective theory for deformed nuclei*, T. Papenbrock, Nucl. Phys. A **852**, 36 (2011).
8. *Occupation number-based energy functional for nuclear masses*, M. Bertolli, T. Papenbrock, S. Wild, Phys. Rev. C **85**, 014322 (2012).
9. *Chiral three-nucleon forces and pairing in nuclei*, T. Lesinski, K. Hebeler, T. Duguet and A. Schwenk, J. Phys. G: Nucl. Part. Phys. **39**, 015108 (2012).

Conference Proceedings

10. *Lowest-order contributions of chiral three-nucleon interactions to pairing properties of nuclear ground states*, T. Duguet, T. Lesinski, K. Hebeler, A. Schwenk, Proceedings of the International Niigata 2010 Symposium “Forefronts of Researches in Exotic Nuclear Structures,” Mod. Phys. Lett. A **25**, 1989 (2010).

Talks

Michael Bertolli (MB), Thomas Lesinski (TL), Thomas Papenbrock (TP)

A. Talks and presentations at meetings

1. “Shell model based energy functional for nuclear masses,” From quarks to the Nuclear Many-body Problem, Oslo, May 21-24, 2008 (TP).
2. “Physics of nuclei” (three lectures) National Nuclear Physics Summer School 2008, Washington D.C., June 23-27, 2008 (TP).
3. “Nuclear structure from light to heavy,” (four lectures) TRIUMF Summer Institute 2008, Vancouver BC, August 4-8, 2008 (TP).
4. “Energy Functional for the 3-level Lipkin Model,” 7th CNS-EFES Summer School. University of Tokyo, Tokyo. 26 Aug. – 01 Sept. 2008 (MB).
5. “Energy functional for the three-level Lipkin model,” The 3rd LACM-EFES-JUSTIPEN Workshop, ORNL, February 23-25, 2009 (MB).
6. “Non-empirical Nuclear Pairing Functional,” LACM-EFES-JUSTIPEN workshop, February 25, 2009, Oak Ridge, TN, USA (TL).
7. “Nuclear Energy Functionals for the 3-level Lipkin Model and the sd-shell,” APS April Meeting, Denver, CO, 02-05 May, 2009 (MB).
8. “Energy Functionals for Nuclear Masses in the sd-shell,” Poster at the 8th Annual Summer School on Exotic Beam Physics, Lawrence Berkeley National Lab, Berkeley, CA, 03-08 August, 2009 (MB).
9. “Non-empirical Pairing Functional from low-momentum two-and three-body interactions,” JUSTIPEN-EFES workshop, December 9, 2009, RIKEN Nishina Center, Wako, Japan (TL).
10. “Nuclear many-body theories” (five lectures), A School on Topics in Nuclear Many-Body Theory, from Lattice QCD to Nuclei, January 4-9 2010, Gala, Norway (TP).
11. “Global mass model in the shell model,” The 4th LACM-EFES-JUSTIPEN Workshop, Oak Ridge, March 15-17 2010 (MB).
12. “Model independent computation of atomic nuclei: status and perspectives,” The INT at 20 years: The Future of Nuclear Physics and its Intersections, Seattle, WA, July 1-2, 2010 (TP).

B. Invited colloquia and seminars

13. “Frontiers of the nuclear quantum many-body problem,” Physics colloquium, University of Tennessee, October 13, 2008 (TP).
14. “Non-empirical Pairing Functional from low-momentum two-and three-body interactions,” NSCL theory seminar, October 20, 2009, Michigan State University, East Lansing, MI, USA (TL).

15. “Non-empirical Pairing Functional from low-momentum two-and three-body interactions,” UT Nuclear Physics seminar, November 9, 2009, University of Tennessee, Knoxville, TN, USA (TL).
16. “Non-empirical Pairing Functional from low-momentum two-and three-body interactions,” INT seminar, December 17, 2009, Institute for Nuclear Theory, Seattle, WA, USA (TL).
17. “Towards ab-initio theory of heavy nuclei, TRIUMF colloquium, April 19, 2010, TRIUMF,” Vancouver, BC, Canada (TL).