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Competing degrees of freedom in nuclear structure theory
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Final report for 1999-2002

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This is a final report on scientific progress supported in the years 1999-2002.

The central focus of this research was the interplay between three generic classes of degrees of freedom relevant to nuclear structure theory: single-particle degrees of freedom, collective degrees of freedom, and statistical degrees of freedom, which can be thought of as an incoherent mean field or a thermal bath.

The research was very successful, resulting in nine refereed publications, all in Phys. Rev. C, and several conference proceedings.

I divide up the results into three classes:

(1) Random interactions

Recent simulations have shown that random two-body interactions in many-body systems show significant nonrandom behavior. I continued my work on random two-body interactions with a paper on pairing-like behavior, in collaboration with G. Bertsch, D. Dean, and I. Talmi—a paper which since its publication in 2000 has been cited at least 40 times, according to the SPIRES database.

A problem that has not yet been successfully tackled is band structure. Random interactions in boson systems give rise to strong rotational and vibrational signatures, but not in fermion systems. I have tried a number of ensembles but none yield interesting results. This work is ongoing.

(2) Deformation and spin-orbit splitting

A collaboration with J. P. Draayer and two LSU graduate students, V. Gueorguiev and I. Stetcu, has investigated the interplay between deformation and single-particle spin-orbit splitting.

Deformation is a persistent signature of the nuclear many-body system. A compact representation of deformation in nuclei is through the group SU(3), which can be mapped exactly to the many-fermion system. But SU(3) is not an exact symmetry, and many other classic features of nuclei, notably pairing and spin-orbit splitting, mix SU(3) irreps. In fact, in two papers considering *sd*- and lower *pf*-shell nuclides, we found that single-particle spin-orbit splitting was by far the dominant source of mixing of SU(3) irreps. If one removed the spin-orbit splitting in the single-particle energies, then SU(3) became a

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very good symmetry.

This has consequences for modeling realistic nuclear wavefunctions, and in part suggested a 'mixed-mode' approach to shell-model calculations: using SU(3) irreps to encode deformation, and *jj*-coupled single-particle configuations to model spin-orbit splitting (and to a lesser degree, pairing). While reasonably successful, other work by us suggests that using Hartree-Fock states to encode pairing could be even more efficient. Not all of the issues have been resolved, but we are looking at this work as a lead-up to efficient bases for large scale, *ab initio* nuclear structure calculations.

(3) Tests of the random phase approximation

During the period of this grant I worked with an LSU graduate student, Mr. Ionel Stetcu, on nontrivial tests of the random phase approximation (RPA). The original motivation was a suggestion by George Bertsch to use mean-field theory augmented by RPA as a method to systematically calculate binding energies of far-from-stability nuclides, particularly applied to broken symmetries such as deformation. As it turns out, RPA has mostly been tested against toy, one-parameter models such as the Lipkin model. Stetcu wrote a Hartree-Fock+RPA code that worked within an occupation-space shell model representation. The advantage of such a code is that it can be compared directly and fairly to "full" numerical shell model diagonalization. Furthermore, the interactions used are complicated, having several dozen parameters. The result is by far the most direct and rigorous test to date of RPA as a microscopic approximation to a full calculation. Furthermore we allowed arbitrary deformation and treated zero-frequency solutions exactly.

RPA works moderately well, although one should be aware that it can occasionally give poor results. The failures of RPA, however, are *not* the result of the so-called collapse of RPA, which we have found to be an artifact of one-parameter models (this particular result is being written up). We have laid a solid foundation to compare so-called improvements to RPA, such as quasiparticle RPA, renormalized RPA, dressed RPA, etc.; in the future we will test these against exact shell-model calculations and see just how much of an improvement they are over plain RPA. We found that the stability of RPA is rather sensitive to restrictions in the wavefunction; for example, we restricted ourselves to real-values Hartree-Fock wavefunctions but allow the equivalent of imaginary RPA excitations: in some, but not all, cases RPA is unstable because one has not yet found the true mean-field ground state.

Finally, we considered a well-known theorem relating the energy-weighted sum rule to the Hartree-Fock expectation value of a double commutator, a theorem by the way found in most textbooks. Stetcu found that when one has a deformed ground state, or indeed when the Hartree-Fock state breaks any exact symmetry, the standard statement of the energy-weighted sum rule theorem is wrong. He also found the correct statement and confirmed it numerically. To date most applications of RPA have been on spherical nuclides, but as computer power grows there are more and more deformed mean-field calculations and likely to be more applications of RPA to deformed systems. In this case, Stetcu's modified theorem could prove a useful insight.

We plan to continue working on RPA in the near future.

Student Support

Two PhD students at Louisiana State University were supported by this grant: halftime support of Vesselin Gueorguiev, PhD October 2002 (major advisor Professor J.P. Draayer, but nearly all of his thesis work was done in collaboration with myself; two publications resulted and at least one more is in preparation), and full time support of Ionel Stetcu, PhD June 2003 (major advisor C. Johnson) who will go on to a postdoctoral position at University of Arizona with Professor B. Barrett. Stetcu was involved in four publications supported by this grant, and was the main author of two of them.

Publications supported by this grant:

``Generalized seniority from random interactions," C. W. Johnson, G. F. Bertsch, D. J. Dean, and I. Talmi, Phys. Rev. C 61, 014311 (2000). (Note: 40 citations since publication according to SPIRES database.)

``Sum rules regarding the sign problem in Monte Carlo shell model calculations," C. W. Johnson and D. J. Dean, Phys. Rev. C. 61, 044327 (2000).

``Spin structure of many-body systems with two-body random interactions," L. Kaplan, T. Papenbrock, and C. W. Johnson, Phys. Rev. C 63, 014307 (2000).

``SU(3) symmetry breaking in lower *pf*-shell nuclei," V. Gueorguiev, J. P Draayer, and C. W. Johnson, Phys. Rev. C 63 014318 (2000).

``A mixed-mode shell-model theory for nuclear structure studies," V. Gueorguiev, W. E. Ormand, C. W. Johnson, and J. P. Draayer, Phys. Rev. C 65 024314 (2002).

``The random phase approximation vs. exact shell-model correlation energies," I. Stetcu and C. W. Johnson, Phys. Rev. C 66 034301 (2002).

``SU(3) vs. projected Hartree-Fock state," C. W. Johnson, I. Stetcu, and J. P. Draayer, Phys. Rev. C 66, 034312 (2002).

``Scalar ground-state observables in the random phase approximations," C. W. Johnson and I. Stetcu, Phys. Rev. C 66, 064304 (2002).

``Pairing from random interactions," C. W Johnson, Nucl. Phys. A 704 (2002) 276.

``Tests of the random phase approximation for transitions strengths," I. Stetcu and C. W. Johnson, Phys. Rev. C. 67, 043315 (2003). (submitted in 2002).

``Order from chaos in the shell model," C. W. Johnson, Capture Gamma-Ray Spectroscopy and Related Topics: 10th International Symposium (AIP Conference Proceedings 529) p. 518, Stephen Wender, ed., (AIP, Melville, New York, 2000).

"Collectivity, computers, and chaos," Calvin W. Johnson, arXiv:nucl-th/030376; invited talk at Computational and Group Theoretical Methods in Nuclear Physics (to appear in Nuclear Physics A).

Invited Talks Supported by this grant

``Random matrices in nuclear stucture," International Workshop on Advances in the Nuclear Shell Model, Trento, Italy, June 1999.

``Order from Chaos in the Shell Model," Tenth International Symposium on Capture

Gamma-Ray Spectroscopy and Related Topic, Santa Fe, September 1999.

"Pairing from random interactions," Shell Model 2000, RIKEN, Japan, March 2000.

"Order from Chaos in the Nuclear Shell Model," APS Spring Meeting, Long Beach CA, April 2000.

<u>Other talks supported by this grant.</u>

"Orderly spectra from random interaction," Theory Division, Los Alamos National Laboratory, September 1999.

"Order from chaos in nuclei: recent developments," T-16, Los Alamos National Lab, February 2001.

"Order out of Chaos in the Nuclear Shell Model," Triangle Universities Nuclear Physics Seminar, November 2001.