Annual Scientific Report July 2005

"Nuclear Level Densities for Modeling Nuclear Reactions: An Efficient Approach Using Statistical Spectroscopy"

Grant DE-FG-03NA00082

Dr. Calvin W. Johnson, Principal Investigator
Department of Physics, San Diego State University

Summary of Goals of Project

General goals: The general goal of the project is to develop and implement computer codes and input files to compute nuclear densities of state. Such densities are important input into calculations of statistical neutron capture, and are difficult to access experimentally. In particular, we will focus on calculating densities for nuclides in the mass range $A \approx 50$ - 100. We use statistical spectroscopy, a moments method based upon a microscopic framework, the interacting shell model.

Second year goals and milestones: Develop two or three competing interactions (based upon surface-delta, Gogny, and NN-scattering) suitable for application to nuclei up to $A = 100$. Begin calculations for nuclides with A = 50-70.

Key Participants

Dr. Calvin W. Johnson, Associate Professor, Department of Physics, San Diego State University (Principal Investigator)

Dr. Johnson is supported for one month summer salary. He is devoting approximately 25% of his time to the project. (50% during the summer)

Dr. Edgar Teran, Postdoctoral Research Associate, San Diego State University Foundation

Dr. Teran is supported 100% by project funds; his time is 100% devoted to the project.

Major Purchases

No major purchases were made during the reporting period.

Products of this grant

Papers:

-- E. Teran and C. W. Johnson, “A statistical spectroscopy approach for calculating nuclear level densities,” proceedings of the IV International Conference on Exotic Nuclei and Atomic Masses.Mountain Pine, Georgia. September 12-16, 2004, to be published in the "European Physical Journal A Direct"
-- E. Teran and C. W. Johnson, “Behavior of shell-model configuration moments” (in progress and nearly ready for submission).
-- E. Teran and C. W. Johnson, “Mathematical models for configuration densities” (in progress).
-- C. W. Johnson and E. Teran, “The role of the residual interaction in the nuclear level density” (in progress).

Talks and posters:

C. W. Johnson, “Microscopic modeling of nuclear level densities using spectral distribution theory,” Nuclear Theory and Modeling seminar, Lawrence Livermore National Lab, June 2004.
E. Teran, “A Statistical Spectroscopy Approach For Calculating Nuclear Level Densities” (poster) the IV International Conference on Exotic Nuclei and Atomic Masses, Mountain Pine, Georgia. September 12-16, 2004.
C. W. Johnson, “Nuclear level densities from spectral distribution theory,” American Physical Society/Division of Nuclear Physics meeting, Chicago, October 2004.
E. Teran, "Configuration level densities calculations with nuclear spectroscopy” (poster), XXVIII Symposium on Nuclear Physics. Cocoyoc, Mexico. January 4-7, 2005.

Other activity:

Dr. Teran attended the Rare Isotope Accelerator Summer School at Argonne National Laboratory, Argonne, IL. August 8-14, 2004.

Accomplishments to Date and Project Progress

An important idea in what follows: we work in a large, many-body space, but break up the model space into smaller subspaces, which we choose to be shell-model configuration, e.g., $(0f_{7/2})^8$, $(0f_{7/2})^7 (1p_{3/2})^1$, $(0f_{7/2})^6 (1p_{3/2})^2$, etc. We compute moments in each configuration and, as a test, combine those to form *total* moments. We then compute the *partial density* in each configuration, and the total density of states or level density is the sum of partial densities. A second key idea is the functional form used for the partial density. Most authors used modified Gaussians, such as Edgeworth expansions or Cornish-Fisher expansions. Our original proposal was to use binomial distributions because they easily accomodated a nontrivial third moment.

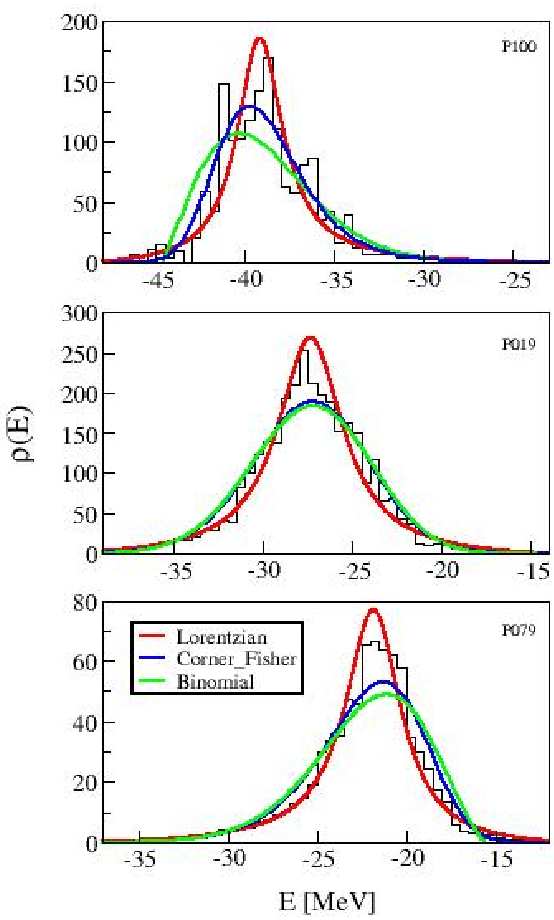
(1) Our work has been slowed by two discoveries. First, we have written a code that computes the require configuration moments, but while validating the code we discovered that the 3rd and 4th configuration moment formulas published in the literature, which are key to efficient large-scale calculations, appear to be incorrect, that is, they do not agree with laborious "direct" calculations (through direct diagonalization of the Hamiltonian matrices; this is limited to fairly small systems). Where the error lies we have not yet found, as derivation of these formulas are very difficult. Second, we have found that the binomial distribution we had proposed to use has only a limited range of applicability, to configurations with a skewness between (roughly) -1 and +1, while many configurations have skewness between -2 and +2.

(2) In addition, we found that other widely used alternatives to binomials, such as the Edgeworth expansion or the Cornish-Fisher expansion, also are deeply flawed.

(3) Instead, we have found a satisfactory alternate distribution to both modified Gaussians and to binomials, which we call the modified Breit-Wigner (MBW) distribution:

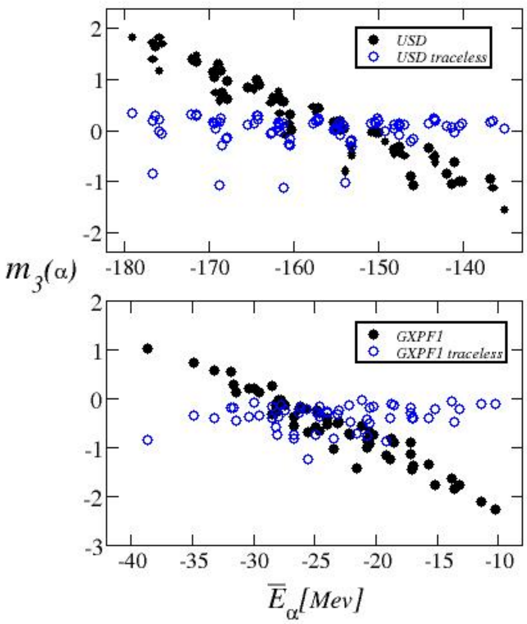
$$\rho_{MBW}(E) = \frac{(E - E_{\min})(E_{\max} - E)}{(E - E_0)^2 + W^2}.$$

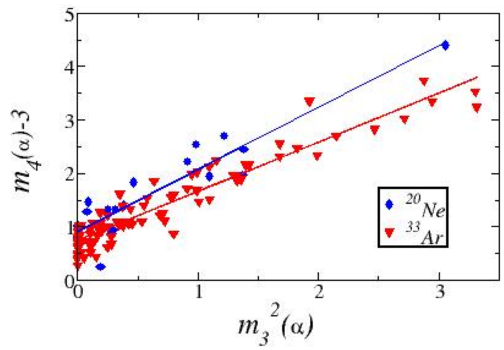
This distribution is positive definite on the range $E_{\min} < E < E_{\max}$, and has analytically calculable moments. The range of moments, including the skewness, is within required limits. Furthermore, by eye it appears to give a better fit to detailed numerical level densities than either binomials or modified Gaussians. (The picture to the right compares exact shell model partial densities with 3 model functions: Binomial, Cornish-Fisher, and Lorentzian = modified Breit-Wigner)



(4) Working with "direct" methods we have made some very useful studies. We have found that there is a close, universal relationship between the third and fourth moments, when properly scaled, which means that in many cases one can avoid computing the difficult fourth moment. Furthermore we find that the second moments also have a universal behavior. This means as we begin to apply our results to realistic systems we can make well-studied approximations that will

enormously speed up our calculations. We are writing up these results as a paper, which will be submitted for publication soon.

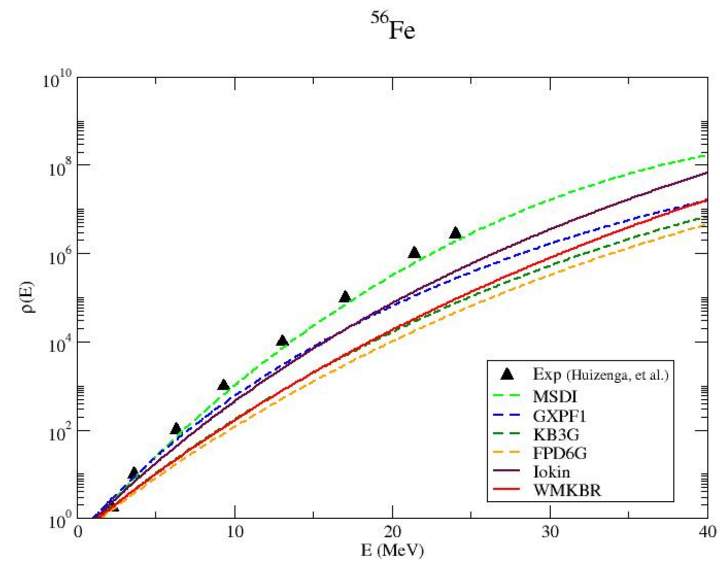




General behavior of configuration moments. *Left*: correlation of third moments (m_3) with centroids; *above*: correlation of 4[th] moments with square of the third moments.

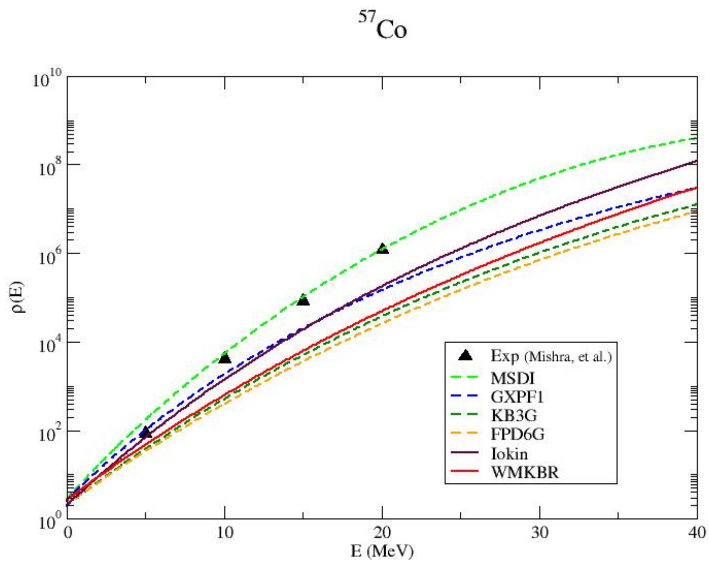
(5) Furthermore, we have found we can exploit these regularities to bypass direct calculation of 3[rd] and 4[th] moments and to speed up calculations. For example, we find that for most configurations, the configuration 3[rd] moment can be approximated just using centroids $\overline{E}_\alpha$ and partial variances $\Gamma_{\alpha\beta}$ (defined in technical appendix).

(6) Despite the above setbacks, Dr. Teran has begun to compare our level densities (using only second moments) with experimental results. He finds that the modified surface-delta interaction provides the best description of experiment.



Right: computation of level density for ^{56}Fe for a variety of different interactions (some in different model spaces). For this calculation we only used Gaussians (no third moments). The Modified Surface-Delta Interaction (MSDI) in the *pf* shell gave the best agreement with experimental data (triangles); note however this could change as one changes the model space.

Right: same as on previous page, but for ^{57}Co. Note the same interaction (MSDI) also yields the best fit to data (triangles).



Summary of progress

We have made significant inroads, although much of it is has been in debugging our original assumptions. Our most important achievements are (1) we have learned that a modified Breit-Wigner distribution is a superior basis for partial densities, much better than previously proposed distributions, including the binomial distribution proposed by Zuker and originally championed by us; and (2) we now have a clear picture how to simplify and speed up our computation of moments. Finally, (3) despite these hindrances, we have started to make significant progress towards our 2nd-year milestones by beginning to compare data against different interactions. Preliminary results suggest the the modified surface-delta interaction works well. Future investigations will see how much of these depends on the mean-field structure of the interaction.

Future plans:

In the immediate future we plan to:

(a) We will now move to testing and validating different interactions by comparing to data. We will begin with the lower *pf*-shell, and then move up in mass, including the $0g_{9/2}$ orbit. Because we have found "shortcuts" in computing moments, we can quickly catch up with our milestones.
(b) We will pay close attention to the mean-field (monopole) structure of the interactions. We have the tools to do this efficiently; we can, for instance, take two different interactions (such as surface-delta and ab initio NN) and force them to have the same mean-field behavior.
(c) In particular, by the end of 2005 we play to have gotten through mass 60 and continued to compare multiple interactions, in particular surface-delta, Gaussian-type interactions (e.g. Gogny), and NN-scattering.
(d) In Fall 2005 we will also revisit the issue of expectation values which will allow us to compute spin-dependence, project out (approximately) spurious center-of-mass motion, and so on.
(e) In January-March 2006 we will apply our calculations to mass 80.

(f) In April-summer 2006 we will apply our calculations to the mass 90-100 regime. We will finish by compiling a library of our results.

Technical Notes: Let **H** be the many-body Hamiltonian. Let P_a be a projection operator on a subspace (a configuration). Then we define the configuration moments as follows:

The dimension of configuration a is $D_a = \mathrm{Tr}\, P_a$;

The *centroid* of configuration *a* is $\overline{E}_a = \frac{1}{D_a} Tr P_a \mathbf{H}$;

The 2nd central configuration moment is $\sigma_a^2 = \frac{1}{D_a} Tr P_a \left(\mathbf{H} - \overline{E}_a\right)^2$;

The 3rd central configuration moment is $\mu_a^{(3)} = \frac{1}{D_a} Tr P_a \left(\mathbf{H} - \overline{E}_a\right)^3$;

The *partial variance* is $\Gamma_{\alpha\beta} = \frac{1}{D_\beta - \delta_{\alpha\beta}} \left[\frac{1}{D_a} Tr P_a \left(\mathbf{H} - \overline{E}_a\right) P_\beta \left(\mathbf{H} - \overline{E}_\beta\right) \right]$.

Finally, one approximate the configuration third moment by $\mu_a^{(3)} \approx \sum_\beta \Gamma_{\alpha\beta} D_\beta \left(\overline{E}_\beta - \overline{E}_\alpha\right)$.