Annual Scientific Report July 2004

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

Grant DE-FG-03NA00082

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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 ≈ 50 - 100. We use statistical spectroscopy, a moments method based upon a microscopic framework, the interacting shell model.

First year goals and milestones: In the first year we proposed to:
(1) Write the basic code, CONMOM. CONMOM reads in the nuclear Hamiltonian, in the form of single-particle energies and two-body matrix elements of the residual interaction, and computes configuration moments of a many-body Hamiltonian, without having to construct, as an intermediary step, the actual many-body Hamiltonian matrix. This code is written in Fortran 90 and can be run on parallel, Beowulf-class machines.
(2) Compute densities for Ti and V isotopes.
(3) Explore efficient computation of moments.

Key Participants

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

Dr. Johnson is supported for two months summer salary. He is devoting approximately 25% of his time to the project.

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

Dr. Teran was a new hire, August, 2003. He is supported 100% by project funds and his time is 100% devoted to the project.

Major Purchases

No major purchases were made during the reporting period.

Publications and Talks

No publications have been submitted at this time, although we have drafts of two papers. The PI (Johnson) has given several talks about preliminary results:

"Microscopic modeling of nuclear level densities using spectral distribution theory," 2004 SSSA Program Symposium, Albuquerque, March 2004.

"Microscopic modeling of nuclear level densities using spectral distribution theory," T-16 seminar, Los Alamos National Lab, March 2004.

"Microscopic modeling of nuclear level densities using spectral distribution theory," Nuclear Theory and Modeling seminar, Lawrence Livermore National Lab, June 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.

(1) We have developed a moments code, CONMOM, and implemented it on a Beowulf parallel cluster. We have also written a code, SUPARB, which reads in the moments, and generates a level density as a sum of binomials.

(2) We have worked assiduously to test and verify the CONMOM code, by comparison with systems sufficiently small that their entire Hamiltonian matrix can be easily handled. Unfortunately in many but not all systems we have a persistent discrepancy in the third and fourth moments. This problem is subtle and has been very difficult to track down. For the very simplest system (particles all in the same orbit) there is no discrepancy. In addition, it turns out for large systems, the *total* third and fourth moments are nearly correct, as they are dominated by contributions from products of the first and second configuration moments. (See Technical Note at end.) With some nontrivial effort we have written codes to test individual configuration moments. We have concluded the error is not in implementation but appears to be an error in the published formulas we have used (which are very complicated and could be subject to typographical errors, etc.; we have contacted at least one of the authors, but since they were derived 30 years ago we were not able to make much progress that way). Such formulas are also extremely difficult to derive, using very obscure methods. Nonetheless we are working to rederive the moments. Until we have 100% confidence we are reluctant to publish results.

(3) Despite problems with the moments, we have gone ahead and computed densities for ^{44}Ti, ^{51}V and other nuclides; these "dry runs" give us a chance to test timing, as well as give us a preliminary comparison to known experimental data (because we know that at moderate excitation energy the results are insensitive to the third moments; unfortunately, until we can describe the low-energy results with third moments it is difficult to publish these preliminary results) . Specifically, we have

worked in a model space $1s_{1/2}$-$0d_{3/2}$-$0d_{5/2}$ + $1p_{1/2}$-$1p_{3/2}$-$0f_{5/2}$-$0f_{7/2}$ with an interaction supplied to us by Dr. W. E. Ormand of Lawrence Livermore National Lab; we have computed normal and abnormal parity densities including up to 3-particle, 3-hole excitations. We have found the densities not only as function of excitation energy E_x but also as angular momentum J. (We could also easily find the densities as a function of isospin.) We have computed information on contamination from spurious center-of-mass motion but have not yet used that to separate out such contamination.

(4) This study has already yielded useful information. For example, computing the third moments take significantly more time than the second moments. Although we are concerned about the accuracy of our third moments, we have reason to believe that they only need to be accurate at low energy (see Technical Note at end). If this is true, we can make our calculations much more efficient by only computing third moments up to a certain energy.

(5) We have done a preliminary comparison of the calculated level densities against experimental results in the lower *fp* shell. Our calculations are somewhat low (roughly a factor of 2) compared to experiment. The discrepancy could be due to (a) erroneous third moments (unlikely to be signficant), (b) choice of interaction, or (c) an inappropriate model space (for example, we leave out the $0g_{9/2}$ orbit).

(6) Because of our experience with the third moments, we have done some calculations comparing the relative importance of first and second moments. To lay the background for this work, it is necessary to know that the standard approach to level densities are almost always some variation of the Bethe Fermi gas approach, which is an independent-particle model with the residual interaction added afterwise in a piecewise and somewhat *ad hoc* fashion. Our study shows that the residual interaction is important at least up into moderate excitation energy, which means one must be cautious in applying Fermi gas models that are cavalier with the residual interaction. The discrepancy can be anywhere from a factor of two to ten. We are currently attempting to make a more systematic study. Note: once we have reliable *third* moments, we will do a similar study, although we known from adjusting the third moment that they have a significant effect only at low excitation energy (but that is important for determing the “ground state” energy).

(7) We have made contact with Gary Mitchell’s group at NCSU, which is doing experimental measurements of level densities. We have also spent time at Livermore and Los Alamos, talking with the applied physics groups interested in level densities, and gotten helpful feedback from them. For example, *everyone* is, unsurprisingly, interested in the actinides. The model space for the actinides is very large and challenging, but if we can devise a satisfactory scheme for computing moments efficiently, that is, only computing the low-energy third moments, they may become tractable.

Summary of progress

We have made significant progress to our milestones. This despite the fact that Dr. Teran only began work on the project in August, 2003, and spent the remainder of 2003 learning the basics of our methodology. We have a serious technical issues, in the discrepancy of the third moments, but we have developed computational tools to help us track it down and resolve it. Aside from the reliability of the third moment, we are "on track" with our milestones. In addition, we have developed significant experience in the codes and model spaces and are well on our way to understand exactly the relative importance of the configuration moments at any given excitation energy.

Future plans:

In the immediate future we plan to:

(a) Solve the discrepancy with the third and fourth moments. This will be done through a combination of rederiving the published formulas and careful examination against exact cases (since it is likely to be misplaced factors of two, delta functions, etc.)
(b) Look again at our model space for the lower *pf*-shell, include the $0g_{9/2}$ orbit, and recompute level densities.
(c) We will start to compile libraries of different interactions and compare their results for the lower *pf*-shell.
(d) Continue our study of approximating moments, especially 3^{rd} moments at moderate excitation energy.

(see next page for Technical Note)

Technical Note: 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 *total* dimension is $d = \sum_a d_a$;

the *total* centroid is $\overline{E} = \frac{1}{d} Tr\mathbf{H} = \frac{1}{d} \sum_a d_a \overline{E}_a$;

and, finally, one can the *total* third central moment in terms of these configuration moments:

$$\mu^3 = \frac{1}{d} Tr\left(\mathbf{H} - \overline{E}\right)^3 = \frac{1}{d} \sum_a d_a \left(\mu_a^3 + 3\left(\overline{E}_a - \overline{E}\right)\sigma_a^2 + \left(\overline{E}_a - \overline{E}\right)^3\right).$$

Even if there are errors in the μ's, they tend to cancel out, so that the total third moment is numerically very close to the correct answer, which makes it difficult to track down the problem.

On the other hand, it is the fact that the μ's can be erroneous that suggests one might be able to speed up the calculation by approximating or eliminating the μ's at higher excitation energy.