LA-UR- 04-6889

Approved for public release; distribution is unlimited.

Title: Improved Nuclear Level Densities via Identification of Spurious Levels

Author(s): U. Agvaanluvsan, G.E. Mitchell, D. Dashdorj, C.M. Frankle, S.F. Lokitz, J.F. Shriner, Jr.

Submitted to: International Conference on Nuclear Data for Science and Technology

Improved Nuclear Level Densities via Identification of Spurious Levels

U. Agvaanluvsan*, G. E. Mitchell†, D. Dashdorj*, C. M. Frankle**, S. F. Lokitz† and J. F. Shriner, Jr.‡

*North Carolina State University, Raleigh, NC 27695
and Lawrence Livermore National Laboratory, Livermore, CA 94551
†North Carolina State University, Raleigh, NC 27695
and Triangle Universities Nuclear Laboratory, Durham, NC 27708
**Los Alamos National Laboratory, Los Alamos, NM 87545
‡Tennessee Technological University, Cookeville, TN 38505

Abstract. An accurate value of the nuclear resonance spacing is crucial for determination of level densities. Level densities are key input for the calculation of nuclear reaction rates and cross sections. This paper discusses various effects that can adversely impact the average level spacing, with a special emphasis on the issue of quantum number assignment. The most striking property of spacings of resonances with the same quantum number is level repulsion. We investigate how a simple test based on level repulsion can be used in the identification of spin misassingment and provide new experimental verification of the proposed test. Proton resonances obtained in the ^{44}Ca+p reaction are used as an example. In addition, s-wave neutron resonances in the ^{238}U+n reaction are considered.

INTRODUCTION

Nuclear level densities are one of the most important components for calculating nuclear reaction rates and cross sections. The average level spacing along with known low lying discrete levels determine the level density parameters used in codes such as GNASH, EMPIRE, STAPRE. The accuracy of the output of such codes, nuclear reaction rates and cross sections, depends on how well input parameters are determined. Therefore, accurate values of the average spacings are crucial.

Experimental data for level density are clustered into two excitation energy regions, the first from measurement of low-lying discrete levels and the second from resonances just above the neutron or proton binding energy. The density of s-wave resonances is calculated by taking the inverse of the average neutron (proton) s-wave resonance spacing, often denoted by D. This value is used for the calculation of the total level density ρ_{Bn} near neutron (proton) binding energy. The level densities between discrete levels and ρ_{Bn} are interpolated using various phenomenological level density formulae. For level densities obtained by such interpolation, ρ_{B_n} serves as a benchmark point. Therefore it is important to obtain D in the first place.

The level spacing D is the energy interval under consideration divided by the number of resonances in that energy interval. The energy interval is rather well determined within the experimental energy resolution. However, the number of resonances is subject to mistakes. The two main sources of mistakes are 1) missing resonances because of experimental limitation, 2) assigning an incorrect quantum number to a resonance. For the missing level problem, the standard approach assumes that the underlying distribution for the reduced witdth is a Porter-Thomas (PT) distribution. One assumes that the weakest levels are missed and the PT distribution is modified according to this assumption. The solution to the maximum likelihood function is determined by iteration which provides the missing fraction of the observed sequence [1]. The PT distribution follows from the fact that a sequence of nuclear resonances, grouped by their quantum numbers, obey the predictions of the Gaussian Orthogonal Ensemble (GOE) version of Random Matrix Theory (RMT).

The method based on the reduced widths works well in the absence of non-statistical effects. Non-statistical phenomena such as doorway states effect the average value of the reduced widths and thus the width approach becomes unreliable. In order to improve the reliability of the analysis, another approach based on the measured spacing distributions has been considered. Using the principle of maximum entropy, we have obtained the probability distribution for imperfect eigenvalue sequences. The two methods used to determine the missing levels were compared in a recent paper [1]. The method has also been extended to other statistics by Bohigas and Pato [2].

In the present paper, we focus on the other major problem, that of quantum number misassignment. For neutron resonances the assignment issue is dealt with using probabilistic Bayesian arguments based on the resonance widths. In the present work we adopt a different approach to deal with the spurious level problem by considering the resonance spacings.

Historically, the effect of spurious resonances on neutron resonance sequences has been investigated by Rainwater and collagues at Columbia [3, 4] using the Dyson F-statistic. The Dyson F-statistic is defined as

$$F_i = \sum_j f((E_j - E_i)/L), \tag{1}$$

where

$$f(y) = \begin{cases} \frac{1}{2}\ln\left|\frac{1+(1-y^2)^{1/2}}{1-(1-y^2)^{1/2}}\right| & : \quad |y| < 1 \\ 0 & : \quad |y| \geq 1 \end{cases} \tag{2}$$

For $L = nD$, where n is some selected number, the expectation value of F_i for a resonance with the correctly assigned quantum number

$$< F_i >= n - \ln n - 0.656, \tag{3}$$

with the standard deviation

$$\Delta F_i = [< F_i^2 > - < F_i >^2]^{1/2} = \sqrt{\ln n}. \tag{4}$$

For a spurious resonance $< F_i > \approx n$. In order words, the spurious resonance will appear as a fluctuation in F of order $\ln n$ which need to be compared to the standard deviation $\sqrt{\ln n}$. The spurious resonances appear as peaks while missing resonances appear as dips. This test was designed to provide the purity test and can be used to improve the quality of level sequences. Several others applied the test to the experimental data with varying success: see for example [5] and [6]. This test works better for a large value of n. The relatively small size of the nuclear resonance sets limits the application of this approach.

We adapt a simple approach based on level repulsion. The most striking characteristic of the spacing distribution of the GOE sequence is level repulsion. In other words the probability that two resonances with the same quantum number have the same energy is negligibly small. Since states of the same symmetry do not occur in close proximity, one can use small spacings as a signature of misassignment. If some of the resonances in a set of resonances with given spin and parity have been misassigned, the experimental data set will be composed of two or more symmetry classes. The issue is to identify these spurious resonances. The mixture of different symmetry classes destroys the level repulsion. By studying anomalies in the resonance spacings one can use probabilistic arguments concerning the quantum number assignments. The method will be discussed and then applied to proton and neutron resonances. In this paper, we consider the $1/2^+$ and $1/2^-$ proton resonance sets from the ^{44}Ca+p reaction and $1/2^+$ neutron resonances from the ^{238}U+n reaction. The proton resonance sets are used to demonstrate the successful application of the level repulsion analysis discussed in the following section.

DATA AND ANALYSIS

For each resonance the energy E and the spin and parity J^π are determined. Here we focus on the energies E_i of resonances $i = 1, \ldots, N$ for a sequence of N resonances. One defines a dimensionless parameter x as

$$x_i = \frac{E_{i+1} - E_i}{D}, \tag{5}$$

where the average spacing D is $D = (E_N - E_1)/(N - 1)$.

Assuming that the nuclear resonances follow the predictions of the GOE, the spacing distribution of resonances is described by a Wigner distribution

$$P(x) = \frac{\pi x}{2} e^{-\pi x^2/4}. \tag{6}$$

The properties of this distribution can be used to test the quality of experimental data. Very large and very small spacings are both unlikely; for example, the probabilities for $x \geq 3$ (large spacings) and $x \leq 0.04$ (small spacings) are ≈ 0.001. Very large spacings may indicate missing resonances while anomalously small spacings may indicate that one of the two resonances separated by that spacing may be spurious. Fig. 1 illustrates the relative probability of small spacings for the Wigner distribution (6). The percentage values are obtained in a straigthforward calculation by integrating the distribution up to the given value of x.

In Fig. 2, spacing data for $1/2^+$ and $1/2^-$ resonances in proton scattering data from the ^{44}Ca+p reaction is shown. The inverse parameter $1/x$ of the spacing parameter x is plotted in order to emphasize the small spacings. The resonance sets include data obtained in several experiments [7, 8, 9, 10] performed at the High Resolution Laboratory of the Triangle Universities Nuclear Laboratory prior to the most recent and compherensive experiment. The horizontal lines indicate the 0.1, 1, and 2% probability values (99.9, 99, and 98% confidence intervals) for the given $1/x$ parameter. For example, as shown in the upper graph, there are three spacings that have a

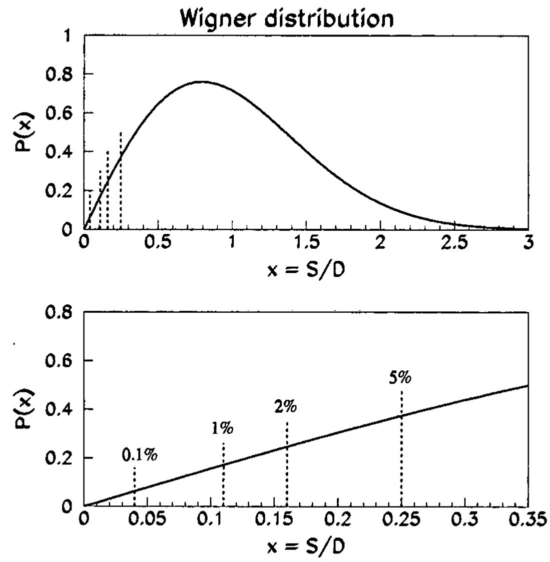

FIGURE 1. The relative probability of small spacings for a Wigner distribution. The upper panel shows the Wigner distribution (solid line) where the probability of small spacings at various x is indicated (dashed lines). The enlargement is shown in the lower panel with the corresponding percentage value.

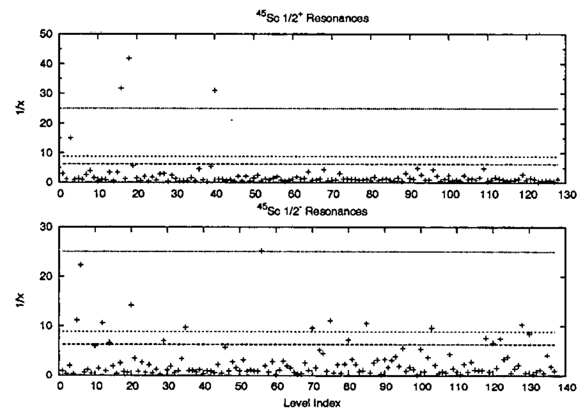

FIGURE 2. The $1/2^+$ and $1/2^-$ resonance spacings from the ^{44}Ca+p reaction with previously available data

$1/x$ value that exceeds the 0.1% chance limit and probabilistically there is 99.9% confidence that a resonance has been misassigned. The situation is even more severe in the case of $1/2^-$ resonances as indicated by the significant number of anomalously small spacings.

These data suggested that many p-wave resonances may have been misassigned. Since these data were a combination of several experiments performed over a period of years, a new and more comprehensive experiment has been performed recently.

The proton beam impinged on a 95.9% enriched ^{44}Ca target with thickness 1.1 - 1.5 μg/cm^2. The experimental resolution was $\sim$ 300 eV. More than 800 hundred resonances were observed. The experimental data were fit with the R-matrix code MULTI6 which uses the formalism of Lane and Thomas [11]. The experimental details and equipment set-up are discussed in Refs. [12, 13]. The R-matrix fit to the elastic and inelastic proton yield for the ^{44}Ca+p experiment is shown in Fig. 3.

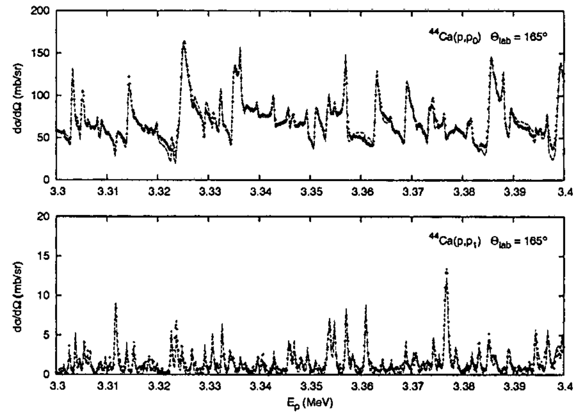

FIGURE 3. The R-matrix fit for the ^{44}Ca+p data

As a result of the improved experimental conditions and better energy resolution compared with the previous experiments, the spin and parity assignments have also improved. In the latest experiment 375 new resonances were observed. About quarter of the previously observed resonances were assigned different quantum numbers. Many of the reassignments correspond to cases that show themselves as anomalies in the $1/x$-test. The result of the new experiment is shown in Fig. 4. Comparing the lower panels of Fig. 2 and Fig. 4, a striking difference can be observed, especially for the $1/2^-$ resonances. This validates the utility of this relatively simple test as a measure of data quality and as a method of identifying probable misassignments.

The final results for the level density in ^{45}Sc are $\rho = 127^{+7}_{-8}$ MeV^{-1} for $1/2^+$ resonances and $\rho = 132^{+8}_{-9}$ MeV^{-1} for $1/2^-$ resonances.

We applied the same test to the $1/2^+$ resonances in the ^{238}U+n reaction [14, 15]. Because of large penetrability difference in s- and p-wave resonances for heavy nuclei, fewer p-wave resonances are observed in neutron scattering experiments. Therefore the effect of spurious levels is less dramatic in neutron resonances than for proton resonances, as demonstrated in Fig. 5. As expected the s-wave resonances for ^{238}U have very few spurious levels.

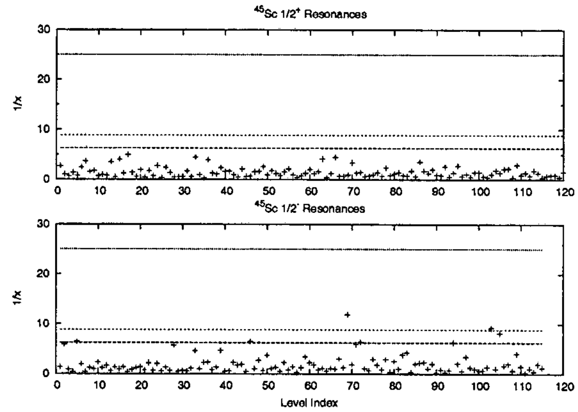

FIGURE 4. The $1/2^+$ and $1/2^-$ resonance spacings in ^{44}Ca+p after the new experiment performed

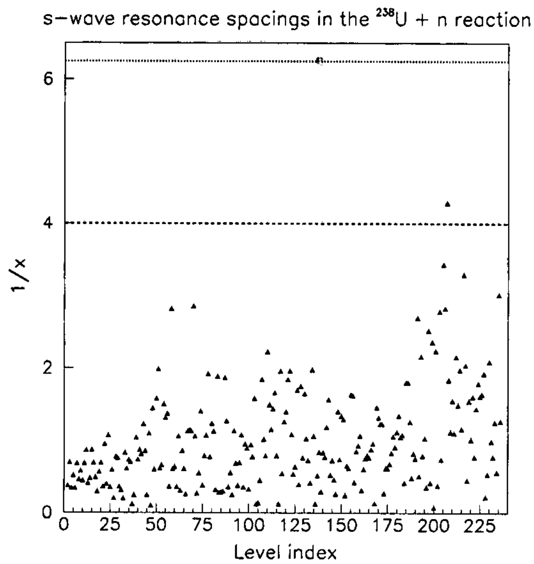

FIGURE 5. The $1/2^+$ resonance spacings in the ^{238}U+n reaction

CONCLUSION

The test based on the level repulsion provides a simple alternative to the purity studies of neutron and proton resonance sequences. Examination of the anamolously small spacings identifies many but not all of the misassigned quantum numbers.

ACKNOWLEDGMENTS

This work was supported by in part by the U.S.Department of Energy Grants No. DE-FG03-03NA00076 and No. DE-FG02-97-ER41042. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory and Los Alamos National Laboratory under contract Nos. W-7405-ENG-48 and W-7405-ENG-36.

REFERENCES

1. Agvaanluvsan, U., Mitchell, G. E., Shriner, J. F., Jr., and Pato, M., *Nucl. Inst. Meth.*, **A498**, 459 (2003).
2. Bohigas, O., and Pato, M. P., *Phys. Lett. B*, **595**, 171 (2004).
3. Liou, H. I., Camarda, H. S., Wynchank, S., Slagowitz, M., Hacken, G., Rahn, F., and Rainwater, J., *Phys. Rev. C*, **5**, 974 (1972).
4. Liou, H. I., Camarda, H. S., and Rahn, F., *Phys. Rev. C*, **5**, 1002 (1972).
5. Monohan, J. E., and Rosebzweig, N., *Phys. Rev. C*, **5**, 1078 (1972).
6. Mehta, M. L., *Random Matrices*, Academic Press New York, 1991, second edn.
7. Wilson, W. M., Bilpuch, E. G., and Mitchell, G. E., *Nucl. Phys. A*, **255**, 262 (1975).
8. Shriner, J. F., Jr., Bilpuch, E. G., Westerfeldt, C. R., and Mitchell, G. E., *Z. Phys. A*, **305**, 307 (1982).
9. Shriner, J. F., Jr., Whatley, K. M., Bilpuch, E. G., Westerfeldt, C. R., and Mitchell, G. E., *Z. Phys. A*, **313**, 51 (1983).
10. Smith, B. W., Ph.D. thesis, Duke University (1989).
11. Lane, A. M., and Thomas, R. G., *Rev. Mod. Phys.*, **30**, 257 (1958).
12. Lokitz, S. J., Mitchell, G. E., and Shriner, J. F., Jr., *Phys. Lett. B*, **8**, 195 (2004).
13. Lokitz, S. J., Ph.D. thesis, North Carolina State University (2004).
14. Olsen, D. K., et al., *Nucl. Sci. Eng.*, **69**, 202 (1979).
15. Olsen, D. K., et al., *Nucl. Sci. Eng.*, **94**, 102 (1986).