

Statistical Spectroscopy for Neutron-rich Light Nuclei

K. Kar

Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Calcutta 700064, India

Abstract. A statistical framework for nuclear spectroscopy and strength distributions for nuclear excitations and decays has been formulated over the years built on the initial ideas of the use of random matrix theory in shell model spaces. In this spectral distribution theory, statistically averaged forms for the nuclear level density and excitation strength distributions are obtained and making use of the group theoretical structure of the shell model spaces, the averages are evaluated. They avoid diagonalisation of the Hamiltonian in many particle spaces and they are useful for problems of astrophysics. This article describes the application of spectral distribution theory to neutron-rich light nuclei.

1 Introduction

The shell model has been extremely successful in calculating the structure of light spherical nuclei. Using a (1+2)-body realistic interaction the model sets up the matrix for the Hamiltonian in the many particle space with fixed angular momentum and isospin and then diagonalises it to give the energy eigenvalues and the wavefunctions. It can also calculate the transition strengths for different excitation and decay operators using the wavefunctions. The applications of the shell model to the *sd*-shell using many effective interactions, in particular the Universal *sd*-interaction [1] have been carried out over the last few decades with detailed comparisons with experimental data. The extension of this to the very neutron-rich nuclei was initially a challenge but then with the required modification of single particle wavefunctions and interaction matrix elements one saw good agreement with observed data [2]. In the *fp*-shell substantial improvement was achieved once the basis space was extended to large dimensions and interactions with proper adjustment of the monopole term constructed [3].

The use of random matrices to describe the fluctuation properties of nuclear energy levels was tried out by Wigner and others by constructing many ensembles with specific symmetry properties in the 1950's and continued for the next few decades. A number of reviews are available now [4–7] and comparisons of nearest level spacing, Δ_3 statistic for level sequences with fixed (J, T) and other measures using Nuclear Data Ensemble (NDE) [8] done. This activity got a big boost with the Bohigas-Giannoni-Schmit (BGS) conjecture [9] that the fluctuations observed in the random matrix ensembles with fixed symmetries are

universal and they are seen to be followed by a large number of diverse quantum chaotic systems.

But along with fluctuations one explored the use of random matrix theory for the averaged nuclear properties and wanted to see whether the quantities like the level density, orbit occupancy, transition strength densities and sum rule strengths averaged over ensembles are in overall agreement with observed data. Initially Wigner showed that the level density of Gaussian Orthogonal Ensemble (GOE) has the form of a semicircle as a function of energy. Later French and collaborators constructed the Embedded Gaussian Orthogonal Ensembles (EGOE) and showed that they produce gaussian density of energy eigenstates [10] in better agreement with shell model and data [11]. The spectral distribution theory is involved in deriving expressions for the density of the eigenstates, expectation values and transition strengths for different operators and how they can be evaluated for specific nuclei exploiting the group theoretical basis of the shell model spaces and their subspaces involved. For transition strengths and strength sums detailed comparison of the spectral distribution methods with shell model have been carried out for specific *sd*-shell and *fp*-shell examples using the same two body interactions for both methods for electromagnetic and beta decay transitions [12–15]. A number of reviews also describe the spectral distribution theory and its application in calculating structural properties [7, 11, 16].

In this work we revisit the issue of statistical spectroscopy by spectral distribution methods in the more challenging region of very neutron-rich nuclei. We describe the calculation of the binding energies of neutron-rich nuclei in the *sd*- and *fp*-shells and the evaluation of occupancies and sum rule strengths of excitation operators. These studies are useful for astrophysical applications. Occupancies by spectral distribution theory were successfully used for calculating beta decay rates during stellar collapse in the problem of supernova evolution [17, 18].

2 The Spectral Distribution Theory

The eigenvalue density for the Hamiltonian is seen to be a gaussian by the direct application of the Central Limit Theorem of statistics for the non-interacting case with

$$H = \sum n_i \epsilon_i \quad (1)$$

when one ignores Pauli blocking. Here ϵ_i is the single particle energy of the i -th state. Mon and French showed that the density of states, when averaged over EGOE, is a gaussian asymptotically for a k -body Hamiltonian in shell model spaces with m' valence nucleons distributed over N' single particle states. The asymptotic result follows in the dilute limit with m' much larger than k' and $m/N \rightarrow 0$ [10]. This means that for the interacting case with two body random interactions the gaussian result for density of states is still true once it is averaged over the ensemble. It is seen that things do not change if a (1+2)-body interaction is considered with EGOE for the two body part.

To consider real nuclei one needs to partition the full space into subspaces with fixed isospin denoted by $'T'$. One can also distribute the $'m'$ particles into $'l'$ orbits with (m_1, m_2, \dots, m_l) defining a configuration with a total isospin $'T'$ in the shell model space. In that case the configuration-isospin density $\rho_{\mathbf{m},T}(E)$ multiplied by the dimension of the space $d(\mathbf{m}, T)$ gives the intensity $I_{\mathbf{m},T}(E)$ and when they are added over all the configurations gives back the total intensity denoted by $I_{m,T}$.

There is also an important result obtained by French and Smith where with one-body noninteracting Hamiltonian spread over spherical orbits of multiple shells and decomposing the space into subspaces each with a fixed number of particles excited from the lower to the higher orbits, one gets the envelope of the densities of these subspaces giving the total density of states. This as a function of energy, is seen to be in good agreement with the Bethe level density formula given by the form $\exp(2(aE)^{1/2})$ [7, 19]. This gives a microscopic understanding of the well-known level density formula.

The density $\rho(x)$ (in the $'m'$ particle state) taken as the weight function defines a set of orthonormal polynomial $P_\mu(x)$ given by the relations

$$\sum_{\mu} \rho(x) P_{\mu}(x) P_{\mu}(x') = \delta(x - x') \quad (2)$$

$$\int P_{\mu}(x) P_{\nu}(x) \rho(x) dx = \delta_{\mu\nu}. \quad (3)$$

If $\rho(x)$ is a gaussian, then the polynomials are Hermite. Using the polynomials connected to the energy level density the expectation value of an operator $'K'$ in the energy eigenstate $|E\rangle$ can be written as

$$\langle E|K|E\rangle = \sum_{\mu} \langle K P_{\mu}(H) \rangle^m P_{\mu}(E) = \langle K \rangle^m + \zeta_{K,H}(\sigma_K)(E - \epsilon_1) / \sigma_1 + \dots \quad (4)$$

The rightmost expression in the above equation is called the CLT result which holds when the spectra of both $'H'$ and $'H + \alpha K'$ are gaussians for small values of α [20]. This expression leads to a geometric interpretation of the expectation value as a function of energy E . It shows a linear dependence giving large values for the expectation value in the ground state region if the correlation coefficient $\zeta_{K,H}$ between the operators $'K'$ and $'H'$ is negative and large whereas it gives small values when the correlation coefficient is positive and large. When they are uncorrelated then the expectation value, of course, stays constant with energy. One can also write down configuration-isospin averaged form for the expectation value of the operator $'K'$ for making comparison to real nuclei with fixed (m, T) values.

The transition strength of an operator $'O'$ between the final state $\langle E'|$ and initial state $|E\rangle$ is given by

$$R(E, E') = |\langle E' | O | E \rangle|^2 \quad (5)$$

This when summed over all the final states is equal to the expectation value of the sum rule operator $O^\dagger O$ in the state with energy E' i.e. given by the expression $\langle E | O^\dagger O | E \rangle$.

French and collaborators showed by using EGOE ensembles for both the k -body Hamiltonian and k' -body transition operator and with particle number ' m ' much larger than k and k' , in the dilute limit the bivariate strength density defined as the transition strength $R(E, E')$ multiplied by the density of states in the initial and final spaces, $\rho(E)$ and $\rho(E')$ respectively, becomes a bivariate gaussian asymptotically. This immediately shows that the sum rule strength density $S(E)$ given by the expectation value of the sum rule operator multiplied by the density $\rho(E)$ also has a limiting gaussian form. Thus one has an alternate way of evaluating the sum rule strength other than the polynomial form given above. This involves evaluating a few low-lying sum rule strength moments [7, 16] and dividing the gaussian sum rule strength density by the gaussian level density.

Finally we touch upon the subject of propagation of traces in shell model spaces. Using the group $U(N)$ of unitary transformations among the ' N ' single particle states, one can write the trace of a k -body operator $G(k)$ in the ' m ' particle space in terms of the trace in the much smaller ' k ' particle space. The trace is expressed as the dimension of the space times the average of the operator and then the trace propagation equation becomes

$$\langle G(k) \rangle^m = C_k \langle G(k) \rangle^k \quad (6)$$

where $\langle \dots \rangle^m$ denotes the average in the ' m ' particle space. One can use subgroups of $U(N)$ group and write operators, for example the Hamiltonian, in terms of the scalar of the subgroup for the evaluation of traces. For the isospin $U(N/2) \times U(2)$ subgroup the trace equivalent for the Hamiltonian becomes

$$H(m, T) = \epsilon \mathbf{n} + [(W^0 + 3W^1)/8] \mathbf{n}(\mathbf{n} - 1) + [(W^1 - W^0)/2](\mathbf{T}^2 - 3\mathbf{n}/4) \quad (7)$$

Here the operators \mathbf{n} and \mathbf{T}^2 have eigenvalues m and $T(T + 1)$ respectively.

2.1 Binding energies

In spectral distributions the ground state energy \bar{E}_g is identified by going back to discrete states from the continuous density of states [21]- the integrated area below the total intensity upto the ground state is made equal to the degeneracy of the ground state, d_0 , i.e.

$$\sum_{\mathbf{m}} \int_{-\infty}^{\bar{E}_g} I_{\mathbf{m}, T}(E) dE = d_0/2 \quad (8)$$

The calculation of binding energy in the sd -shell using Wildenthal's Universal sd interaction was done [22] following the earlier work with the Kuo

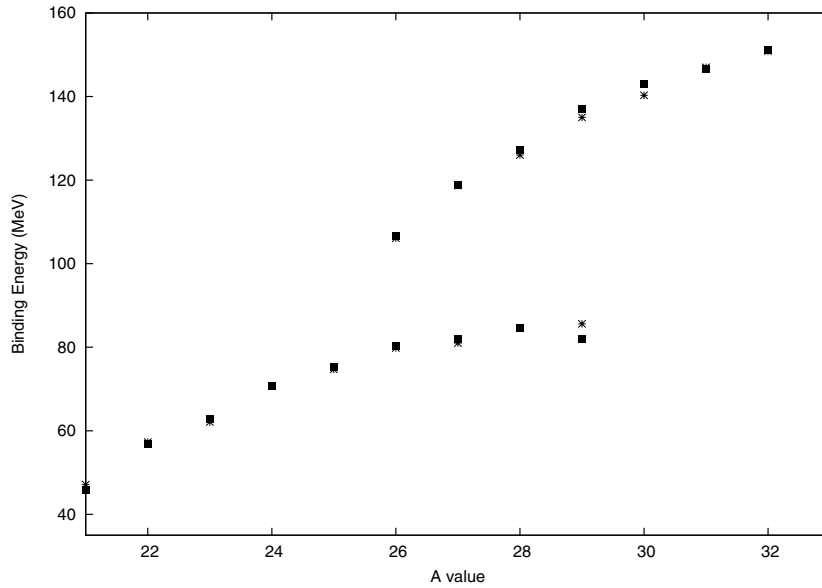


Figure 1. Absolute values of binding energies of isotopes of Ne (the lower ones) and Al (the upper ones) calculated by Spectral Distribution Theory compared to experimental values. The stars stand for the experimental numbers and the filled squares for the predicted values

interaction [23] but taking into account of the correction due to the small but non-zero skewness and excess of the energy density distribution. This was done for nuclei close to the stability line in the sd -shell. Similar evaluation of binding energies for fp -shell nuclei was also carried out using the KB3 interaction in the lower [24] and upper [25] halves of the shell.

Recently spectral distribution theory was applied to calculate ground energies of very neutron-rich nuclei going upto the drip line in some cases [26]. Use of the low-lying excitation spectrum with observed spin as well corrections coming from the third and fourth moments of the density were included. A isospin dependent correction term of $0.3T^2$ was introduced to take care of the lack of knowledge of excited states for nuclei with large neutron excess. Nuclei with neutron number equal to or greater than the proton number (Z) and not exceeding 20 were considered. The 70 cases considered had an average deviation of 0.07 MeV of the predicted binding energy from the observed ones. The RMS deviation is 1.92 MeV which gets reduced substantially when a few nuclei with number of valence particles/holes not large enough are not included. All these results are with ^{16}O as the close core and the Coulomb energy subtracted out. Figure 1 compares the spectral distribution values against the experimental values of the binding energies (taken as positive numbers) for the isotopes of Ne and Al. Figure 2 shows similar calculations done in the lower half of fp -shell

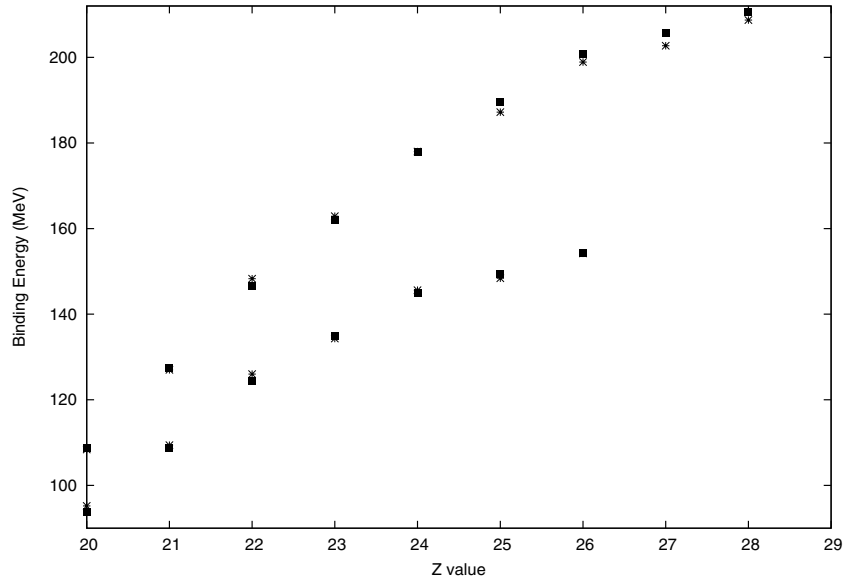


Figure 2. Absolute values of binding energies of fp -shell nuclei with atomic numbers 54 (the lower ones) and 56 (the upper ones). The stars stand for the experimental numbers and the filled squares for the predicted values

for atomic numbers 54 and 56 but in these calculations the very neutron-rich nuclei are not included yet.

2.2 Sum rule strengths and orbit occupancies

We begin with a comparison of M1 strength sum rule by shell model and spectral distribution theory calculations using the moments taken from the shell model. Two examples are considered in the fp -shell-(i) the nucleus ^{46}V with $(J,T=0,0)$ with the shell model space dimension as 814 (ii) the nucleus ^{50}Sc with $(J,T=0,4)$ with the shell model dimension as 5986 [15]. The operators considered are the isoscalar and isovector M1 transitions. The sumrule strengths for the 814 and the 5986 states by shell model are calculated and the matrices for the M1 excitation operator, H and H^2 from all initial states to all possible final states constructed. Then by matrix multiplication the centroid of sumrule strength distribution ($\epsilon_K = \langle KH \rangle / \langle K \rangle$) and its variance ($\sigma_k^2 = \langle KH^2 \rangle / \langle K \rangle - \epsilon_k^2$) are evaluated where K is the sum rule strength operator. Then constructing the gaussian sum rule strength density and dividing it by the gaussian energy density one gets the spectral distribution prediction. Similar comparisons with shell model have been carried out for many large dimensional cases with other excitation/decay operators like isoscalar and isovector $E2$, Gamow-Teller beta decay and good agreement observed.

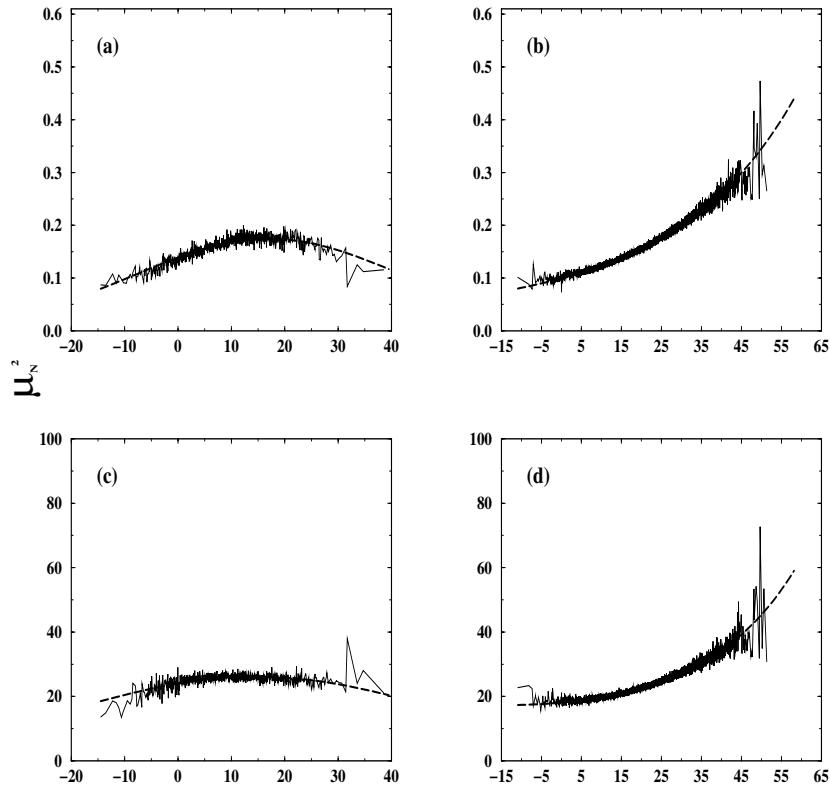


Figure 3. Comparison of $M1$ strength sum by shell model and spectral distribution. The cases marked (a) and (c) stand for the isoscalar and isovector operators respectively for the nucleus ^{46}V and cases marked (b) and (d) stand for the isoscalar and isovector operators respectively for the nucleus ^{50}Sc . Taken from Reference [15]

Figure 3 shows the comparison of sum rule strengths for isoscalar and isovector operators for the nuclei ^{46}V and ^{50}V . It is seen that the strength density form does very well to give the average trends of the detailed shell model results. Thus a spectral distribution theory formulation with four parameters is able to reproduce the average features of the large matrix diagonalisation results.

The expression for the expectation value of orbit occupancy using the polynomial expansion of equation (4) becomes very simple if one considers it averaged over the configuration-isospin space. The correlation coefficient of the orbit occupancy with the Hamiltonian is zero in this space. So the CLT expression for occupancy has only the first term of equation (4) and its energy dependence comes from the ratio of the energy densities in the configuration-isospin and

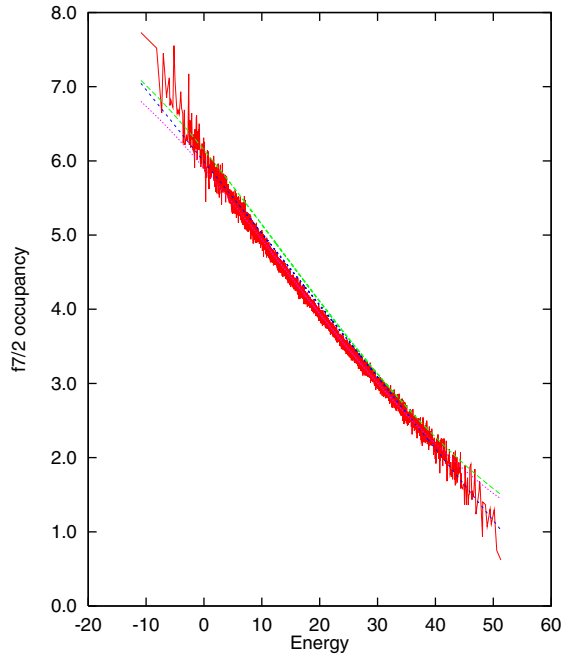


Figure 4. Occupancies of the orbit $f_{7/2}$ for the nucleus ^{50}Sc as a function of energy calculated by spectral distribution compared to shell model values (the fluctuating line). Taken from Reference [7]

scalar-isospin spaces. Figure 4 shows the occupancy of the orbit $f_{7/2}$ for the nucleus ^{50}Sc . The fast fluctuating curve is the shell model prediction whereas the linear curve stands for the spectral distribution polynomial form and the other two are normalised and unnormalised gaussian occupancy density predictions. All three fit the shell model results well but the normalised occupancy density one does it best, as expected.

It is quite simple to calculate the orbit occupancies by spectral distributions as a function of the excitation energy of the nucleus. Figure 5 displays the example of the occupancies of the three sd -shell orbits $d_{5/2}$, $d_{3/2}$ and $s_{1/2}$ for ground states of some isotopes of Ne . For all the cases when the neutron number nears the value 20 i.e. near shell closure, it is clear that the low-lying orbits of the higher shell like $f_{7/2}$ should be included in the calculation for better predictive power.

3 Concluding Remarks

The applications of spectral distribution methods need to be extended to heavier nuclei i.e. beyond the fp -shell with extensive comparison with shell model and

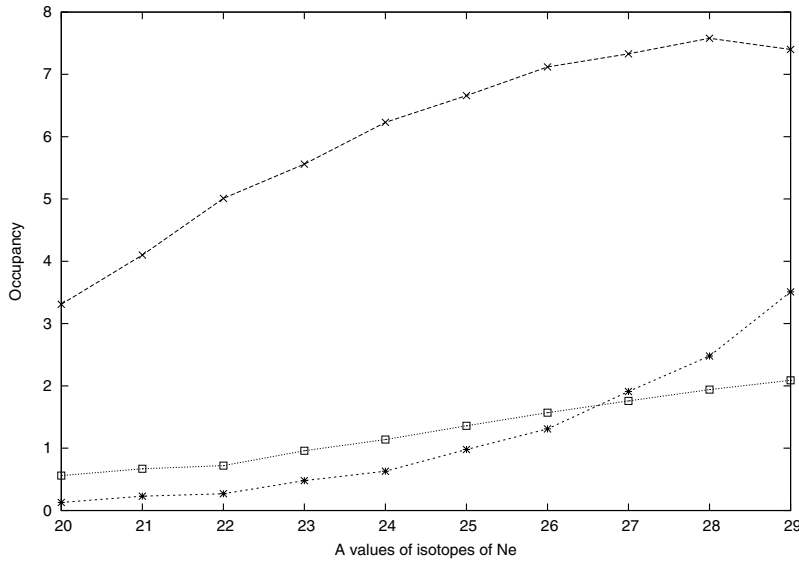


Figure 5. Occupancies of the orbits $d_{5/2}$ (crosses), $d_{3/2}$ (stars) and $s_{1/2}$ (unfilled squares) for isotopes of Neon

other theoretical calculations as well as with experimental data. Particular attention should be paid to some of the very neutron-rich nuclei which are important for astrophysics like the waiting point ones. Different excitation and decay operators need to be considered to get a better insight into the domain of applicability of spectral distribution theory.

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