APPLICATIONS OF SPECTRAL DISTRIBUTION METHODS

Thesis Submitted To
The Maharaja Sayajirao University of Baroda.
In Fulfilment For the Degree of

Doctor of Philosophy

In Physics

By
MISS PRAMILA SHENOY

DECEMBER 1986

S U M M A R Y

In the theory of Nuclear Physics, the Spectral Distribution Methods initiated and developed by J.B. French and Coworkers, occupy a very important place.

Given a nuclear system, conventional spectroscopy aims at constructing the system Hamiltonian matrix and deriving various nuclear properties by diagonalizing the matrix so obtained. The procedure is good enough for nuclei with very few valence nucleons. But for nuclei having large number of valence nucleons this method is not practical because (i) the hamiltonian matrix dimensionalities become forbiddingly large (ii) the computation time increases tremendously, and (iii) the output is too detailed to enable the extraction of useful information.

Spectral Distribution Methods overcome these difficulties because:(i) instead of detailed spectrum of various quantities, they deal with their distributions in energy, configuration etc. (ii) the distribution is determined in terms of its moments, which are the traces of appropriate powers of the hamiltonian, and hence there is no need for explicit evaluation of eigenvalues and eigenvectors, (iii) of the existence of some simplicities like "propogators" and the Central Limit Theorem by virtue of which one needs to calculate only a few lower moments in a space defined by very few particles (usually 2). Moreover, because of the inherent nuclear symmetries and concept of decomposition of space according to these symmetries, the calculations can be further simplified.

Hence we have used spectral Distribution Methods to study and solve various problems related to nuclear properties.

To begin with, one needs proper representation of the nuclear system. The density of eigen-states of a system can draw a very good picture of the system. For this purpose we should have an appropriate representation of the density function. By appropriate we mean that the representation should satisfy certain theoretical and physical norms, besides being reasonably easy to handle mathematically.

In general, there are three known methods of representing a density function: (i) the Pearson system (ii) the series expansion around a well known density in terms of few low order moments and (iii) transformation of variable such that the transformed variable has a known distribution. In this thesis, we have explored the last method. However, for completeness, we have studied all the representations. We have found that, in particular, the Cornish Fisher (CF) expansion gives a very appropriate representation for the density function. It is positive definite for all values of the defining variable despite truncation and is valid for a large range of $\sqrt{_1}$, $\sqrt{_2}$ values. We have compared the CF expansion with other representations and also with the exact results, and found that it fits quite well with the exact results.

Conventionally, the eigenvalues of a Hamiltonian matrix H are obtained by solving the matrix equation $H\psi_i = E_i\psi_i$, where E_i are the eigenvalues and ψ_i are the corresponding

eigenvectors. On the other hand, if we use the spectral Distribution Methods, the discrete eigenvalues can be obtained by numerical integration from the continuous density of states by Ratcliffe's procedure. The averaged i^{th} eigenvalue is given by

$$\frac{i - \frac{1}{2}}{D} = \int_{-\infty}^{E_i} \rho(E)\, dE$$

where $\rho(E)$ is the density of states and D is the dimensionality of the spectroscopic space. Numerical integration has two disadvantages (i) it is tedious and time consuming and (ii) often the calculations give unphysical results because the chosen representation of the density function need not always be positive definite. Moreover, it is found, in general, that the moments obtained from the discrete eigenvalues are not the same as the original moments. This is clearly due to discretization of continuous density.

To avoid these problems, we have developed two methods to calculate eigenvalues of a Hamiltonian matrix, knowing few lower order hamiltonian moments. The first method determines the eigenvalues in such a way that the moments calculated from these eigenvalues are identical to the given moments. The second method is a modification of the Ratcliffe's procedure and involves parametric differentiation of the density function. However, this method takes into account the higher moments only approximately. The CF expansion, besides giving a good fit to the density

function provides a straightforward way to evaluate eigenvalues, taking a complete account of the given moments, usually the centroid E_c, width σ, skewness γ_1 and excess γ_2. We have performed numerical calculations by using the exact shell-model calculation results for all J, T = $\frac{1}{2}$ values in the d-s shell with 5 particles. The eigenvalues obtained by various calculations have been compared with the exact results via their root mean squared deviations. Results obtained by using CF expansion are very encouraging.

Using CF expansion, we have developed a new polynomial expansion for the expectation value of an operator. It is found that in the CLT limit, this expansion reduces to the already existing well known polynomial expansion for expectation values. Besides this, we have applied CF expansion to a ratio of two densities (pertaining to positive difinite operators) and obtained expressions for calculating spherical orbit occupancies. We have performed numerical calculations in the d-s shell with m = 5, J = $\frac{1}{2}$, T = $\frac{1}{2}$, dimensionality D = 109 with Kuo interaction and ^{17}O single particle energies. A plot of occupancies for $d_{5/2}$ and $d_{3/2}$ orbits vs the energy in MeV when compared with the exact shell model results shows that the calculated results are in excellent agreement with the exact results as far as the general trend is concerned.

A set of ground state occupancies forms an important aspect in the theory of nuclear physics and provides a very good clue about the structure of the nucleus. Moreover, these occupancies

can be experimentally measured. Using spectral Distribution methods, we have calculated ground state proton and neutron occupancies for nuclei in the mass range A = 60 - 80. The spectroscopic space for our calculations consists of the $p_{3/2}$, $f_{5/2}$, $p_{1/2}$ and the $g_{9/2}$ orbits with single particle energies 0.0, 0.78, 1.08 and 3.0 MeV respectively. We employed the modified, fully renormalised Kuo-Brown interaction, and the calculations were done in the (p-n) configuration space. It is an experimentally known fact that the proton occupancy structure changes suddenly when the neutron number in the space crosses 12. We have found that the chosen interaction does simulate that change in structure, but it is not found to be as sharp as that given by the experiments.

Besides studying eigenvalue distributions with respect to energy, Spectral Distribution Methods can also be used to evaluate expectation values of various operators as functions of energy. These expectation values are obtained by perturbing the hamiltonian of the system by adding an appropriate function of the operator to it and statistically testing the response of the system as measured by its state density. Various sum rules can then be obtained from these expectation values. Halemane applied Spectral Distribution Methods to the Rayleigh Schrodinger perturbation theory and obtained expressions for varieties of inverse energy weighted sums. We have rederived these expressions by using a different

and simple approach. We have also studied its extension to the CLT limit. From the basic expressions of these sum rules, we have derived detailed analytical expressions for the first and second order perturbation coefficients S_1 (E) and S_2 (E) respectively, in scalar and configuration spaces. We approximated the PW interaction (effective interaction) by a linear combination of Q.Q and Pairing operators and used the expressions of S_1 (E) and S_2 (E) to determine corrections to estimates of ground state energy given by the empirical interaction. The numerical calculations were done in d-s shell with 4 particles. We have found that these methods do give very appropriate corrections to estimates of ground state energy, especially when the calculations are done in configuration spaces.