QUANTUM CHAOS AND CONVERGENCE OF SHELL MODEL ENERGIES

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Statistical properties of complex quantum systems have been studied extensively from various viewpoints. Recently, the detail studies of highly excited states in realistic atomic [1] and nuclear [2] calculations demonstrated that such many-body systems are close to the random matrix theory (RMT) limit although they reveal some deviations which reflect the remnants of the regular structure due to the presence of the mean field, coherent components of the residual interaction and its two-body character. Precise experimental information exists, as a rule, about low-lying states only. However we believe that an intimate relation exists between the low-energy spectroscopy and onset of quantum chaos at high excitation energy and high level density.

The shell model approach is based on the large-scale diagonalization even if one is interested in the low-lying states only. The dimensions of matrices increase dramatically with the number of valence nucleons. Here we suggest a simple approach for calculating energies of relatively low lying states which allows one to reduce those dimensions by orders of magnitude, while keeping high precision of the results. The approach is based on the statistical properties of complicated many-body states. Because of the strong residual interaction, the eigenstates are extremely complex superpositions of simple configurations. However, in contrast to the RMT limit, the stationary wave functions are not fully delocalized in shell model Hilbert space. Due to inherently self-consistent nature of the residual interaction (even if it is extracted in a semiempirical manner), its strength does not exceed the typical spacings between single-particle levels which are determined by the mean field, i.e. by the same original forces. Together with the fact that the two-body forces cannot couple very distinct configurations, this leads to the band-like structure of the hamiltonian matrices in the shell model basis. For such matrices, both mathematical and numerical arguments favor the localization of the eigenstates in Hilbert space.

The generic many-body states in complex atoms or nuclei have a typical localization width which can be measured (in a given basis) in terms of wave-function (information) entropy [2]. Inversely, the simple shell model configurations are packets of the eigenstates. Their strength functions are fragmented over the range of energies, and in the nuclear case, which is close to the strong coupling limit, the typical spreading width can be estimated [3] as , $\approx 2\bar{\sigma}$ in terms of the energy dispersion of a simple configuration $|k\rangle$, $\sigma_k^2 = \langle k|(H - \langle k|H|k\rangle)^2|k\rangle = \sum_{l\neq k} |H_{kl}|^2$. Here H_{kl} are the off-diagonal elements of the residual interaction between the basis states so that the calculation of σ_k does not require any diagonalization. The dispersions of different simple states fluctuate weakly and their mean value $\bar{\sigma}$ can be found without even constructing the full hamiltonian matrix in the spin and isospin projected basis.

The practical method, utilizing the knowledge of a generic energy dispersion $\bar{\sigma}$, was suggested in [4]. The shell model states are grouped into partitions (sets of states belonging to the same particle configuration). Since the states separated in energy by an interval broader than the spreading width are not significantly mixed with the studied state, we truncated the matrix retaining only the partitions whose statistical centroids $\bar{E} = \overline{\langle k|H|k\rangle}$ are closer than 3σ. The spin-isospin projection and the elimination of the center-of-mass admixtures can be done within the truncated subspace only. In order to keep the correct shell model structure, the partitions should be included as a whole. As shown in [4], this simple method allows for the calculation of low-lying energies with sufficient precision in large shell-model spaces. The comparison with available exact results reveals an overlap of the truncated eigenvectors with the exact

ones on the level of better than 90%.

Going beyond the simple truncation, we have studied [5] the convergence of the level energies to the exact values as a function of the increasing dimension n of the diagonalized matrix. As an example we take the ^{51}Sc nucleus where the pf-shell model dimensions of $1/2^-$ and $3/2^-$ states are 13016 and 24474, respectively. Spectroscopic information of this radioactive isotope is only tentative providing an interesting experimental and theoretical problem. Fig. 1 shows the calculated energies of the two lowest $3/2^-$ and $1/2^-$ states for several values of n ranging from $n = 2000$ to the full dimension N. Already the smallest dimension leads to a good agreement within few hundred keV. The solid lines show that in all four cases, as the dimension increases, the running eigenvalue converges very fast and monotonously to the exact result. The convergence is almost pure exponential, $E(n) = E_\infty + A\exp(-\gamma n)$. The exact values of the fitted parameters are given in the figure; typically $A \approx 200 - 300$ keV, $\gamma \approx (6-8)/N$.

The exponential convergence of eigenvalues would be extremely helpful for shell model practitioners. It would make almost redundant the full large scale diagonalization if one is interested in the low-lying states only. Instead, the procedure of calculating the eigenvalues and the eigenfunctions for several increasing dimensions (still far from the full value and therefore easily tractable) would end in determining the exponential parameters and simple extrapolation to the exact result.

At present, the rigorous mathematical theory of convergence is absent. The convergence under consecutive truncations is determined by the type of the matrix and by the unperturbed basis which orders the basis vectors in a certain way. One neeeds to know the weight of small remote admixtures in the stationary eigenvectors. Earlier it was established that the energy behavior of the remote wings of the strength function with high accuracy can be described [3] by an exponential function of energy. This clear manifestation of the localization of the eigenfunctions typical for the banded hamiltonian structures is the origin of the exponential convergence. We considered a number of simple models where it is possible to determine the character of convergence. Roughly speaking, it is the case in the band-like matrices with off-diagonal matrix elements $\langle V^2\rangle$ smoothly decreasing outside the band and the ratio $\langle V^2\rangle/D^2$ approximately constant along the band (D is the level spacing in the remote region).

References

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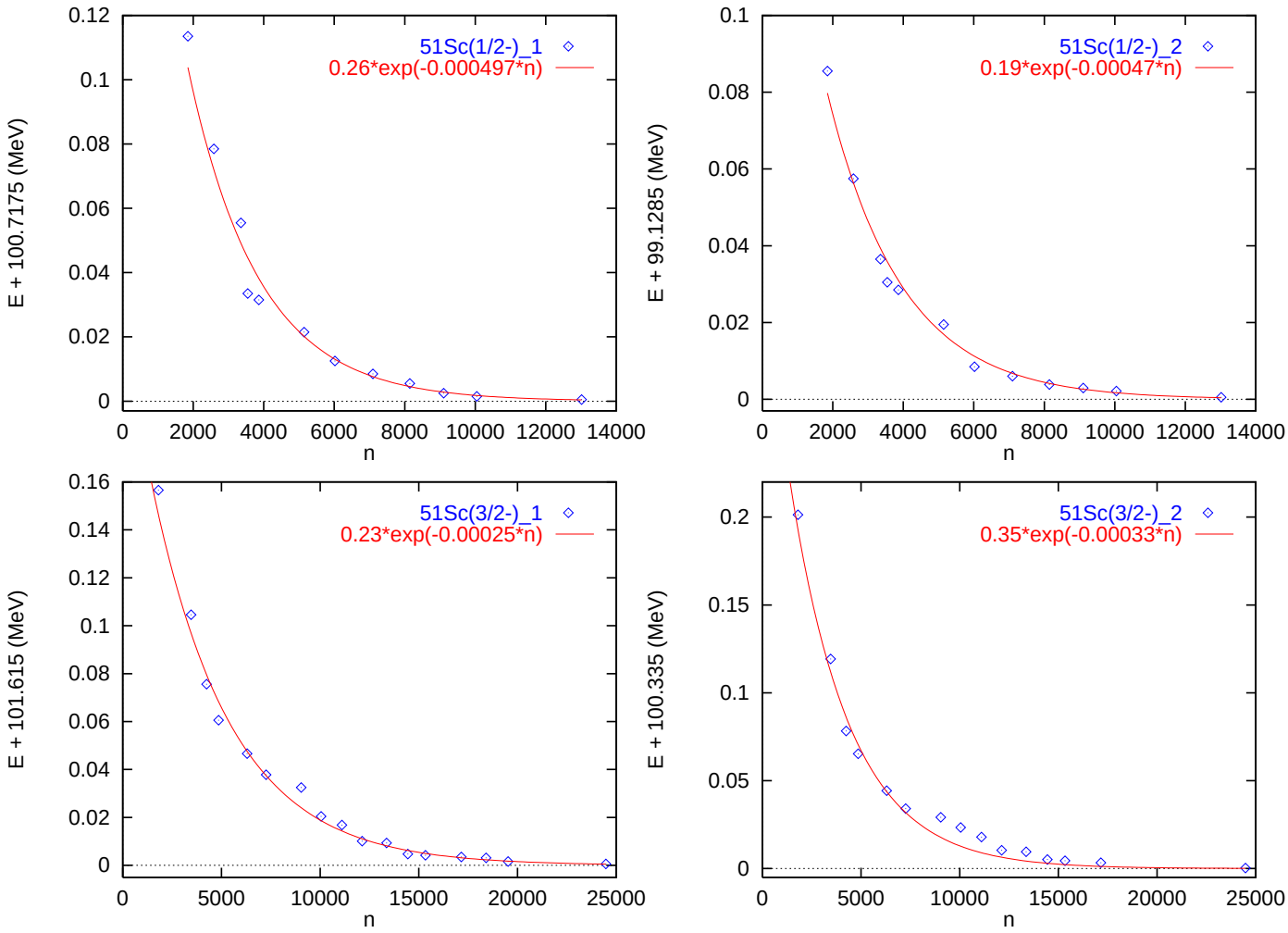

Figure 1:

Figure 1: Energy deviations from the exact pf-shell model results for the lowest excited states $1/2_-$ and $3/2_-$ in ^{51}Sc, diamonds, calculated with the FPD6 effective interaction as a function of the progressive matrix truncation n; solid lines give a fit $A\exp(-\gamma n)$.