Spin- and parity-dependent nuclear level densities and the exponential convergence method

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The knowledge of the nuclear spin- and parity-dependent level densities $\rho(E,J,\pi)$ is important for understanding statistical properties of nuclei and reaction rates. We show that the earlier suggested method of exponential extrapolation, which allows one to find the yrast energy with high accuracy even for very large shell model Hamiltonian matrices, can be combined with the formalism of statistical spectroscopy in order to obtain the reliable level density.

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The knowledge of the level density is an important element of the description of highly excited many-body systems. In application to nuclei, as well as other finite systems such as atomic clusters, the many-body level density determines all statistical properties, both for the discrete spectrum and for reactions. This was recognized more than sixty-five years ago, see Refs. [1,2] and historic references therein, when the statistical approach based on thermodynamic analogies and the Fermi-gas model of the nucleus was developed [3]. The importance of the level densities is obvious, especially in connection to neutron resonances in heavy nuclei and related applications, nuclear reactions in general and advances far from stability in particular, and the astrophysical problem of nucleosynthesis.

The most common semiphenomenological approaches to the problem of the nuclear level density use basically the noninteracting Fermi-gas model of a nucleus with corrections that are needed to take into account the average effects of the shell structure, pairing correlations, and collective excitations associated mainly with the static or dynamical deformation of the mean field [1,4–8]. The residual interaction is fully taken into account in modern large-scale shell model calculations based on a direct diagonalization or, for example, with the use of the Monte Carlo techniques [9–11]; a comparative analysis of these methods was performed in Ref. [12]. One can hope that at not very high excitation energy the finiteness of model space is not crucial because of a relatively low statistical weight of intruder configurations. Furthermore, one can try to smoothly match the exact shell model results to the improved Fermi-gas predictions at higher energies.

As the dimensions of the shell model Hamiltonian matrices grow beyond the directly tractable limits, the approach using the methods of statistical spectroscopy [13–17] is still possible. Moreover, the statistical approach is the most appropriate for answering the questions formulated in statistical terms. Here one needs to build the Hamiltonian matrix and calculate the traces of its moments without an explicit diagonalization. According to the central limit theorem, the distributions of level densities, strength functions, and related quantities are converging to the Gaussian so that the lowest moments are expected to provide sufficient information [17]. The underlying physics can be understood in terms of many-body quantum chaos. Two-body interactions of the fermions in the region of high level density are effectively strong and act essentially at random, as follows from the general analysis [18,19] and from detailed calculations for complex atoms [20] and nuclei [21]. The standard partitioning of Hilbert space according to the particle configurations, which is a usual tool in the construction of the shell model basis, is very convenient here as well since it facilitates the calculation of the traces. The traces can be found for few-particle states and then extended by a combinatorial ''propagation'' to many-body states. Unfortunately, the propagation procedure for the traces including the projection operators for additional quantum numbers is much more complicated [22]. Meanwhile, reliable information on the level density $\rho(E,J^{\pi},T)$ as a function of excitation energy, total spin J, parity, and isospin is highly desirable.

Taking into account only the first two scalar moments of total density seems to be insufficient in cases where the inclusion of many major shells and other shell effects distort the shape of the level density. Recently, Zuker [23] showed that small asymmetries of the level density can be addressed by including the third or/and the fourth static moment(s). In cases where the fluctuations are more pronounced, it was recently shown [24] that after decomposing the shell model space in partitions according to the arrangement of nucleons in single-particle orbits, the total density of states can be found as a sum of the Gaussians G_p on the set of partitions $p=1,2,\ldots,P$ of A valence particles in s single-particle states (e.g., $[n_1(p),n_2(p),\ldots,n_s(p)]$, $A=\Sigma_{i=1}^{s} n_i(p)$),

$$\rho(E)=\sum_{p=1}^{P} D_p G_p(E+E_0-\overline{E}_p,\overline{\sigma}_p), \tag{1}$$

provided that the ground state energy E_0 can be accurately calculated, for example, with the aid of the exponential convergence method [25]. Previously, similar procedures were used to describe the shape of the density, see, e.g., the title of Sec. 3 of Ref. [26]. In Eq. (1), D_p is the total number of states in the partition p, E is the excitation energy, E_0 is the ground state energy, $\overline{E}_p$ and $\overline{\sigma}_p$ are the first (centroid) and second (width) moments, respectively, for each partition. The partition moments $\overline{E}_p$ and $\overline{\sigma}_p$ can be calculated using a

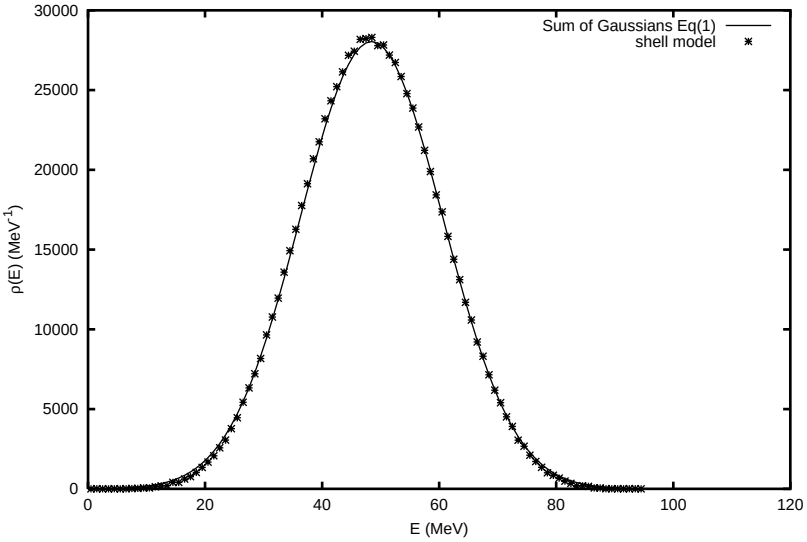

FIG. 1. Shell model density of states compared with the sum of Gaussians approach, Eq. (1), based on partition averages according to statistical spectroscopy.

straightforward method introduced in Ref. [14], see below. The precise knowledge of the ground state energy E_0 is crucial for the application of the partition summation. Figure 1 compares the results of Eq. (1) with full shell model calculations available for the case of $A=12$ valence particles in the sd shell. Partitions have an important advantage of forming an invariant subspace with respect to rotational symmetry and parity. All the results shown in Figs. 1–5 are obtained using the USD interaction of Ref. [27]. In all cases the number of protons equals the number of neutrons and states of all isospins are included.

Previous work on level density mostly stressed only the description of the shape of the density, leaving aside the role of the starting energy. Papers based on Monte Carlo techniques [9–11] use (without emphasizing) the ground state energy, however, they can only include very limited interactions to avoid the sign problem that induces high errors in the value of ground state energy [28]. Kota and Majumbar [29] recognize the importance of knowing the location of the ground state energy. In practice, their approach uses, besides theoretical results related to the shape of the density, set(s) of experimental data, when available.

The total density of states $\rho(E)$ is normally calculated as the first step in many other approaches, including the Fermi-gas model and Monte Carlo method. To obtain the density of levels $\rho(E,J)$ for a given spin J, one usually employs a rescaling procedure based on the statistical distribution of spins, which we describe below. However, we show that this procedure is not sufficiently accurate, especially for the lowest and highest spins.

The approach developed by Jacquemin *et al.* [22,26,30] allows one to calculate exactly shell model centroids $\overline{E}(J)$ and widths $\sigma(J)$ for the level densities at fixed spin J. In principle, the knowledge of the cumulative level number $\mathcal{N}(E,J)=\int_{-\infty}^{E}dE'\,\rho(E',J)$ makes it possible to reproduce the positions of the discrete levels [14]. However, in the lowest part of the spectra this procedure would not work because even the corrected Gaussian approximation does not describe the lowest part of the spectrum that is very far from the centroid. In this situation it is natural to enrich the methods of statistical spectroscopy with information based on the generic properties of complicated (''chaotic'') many-body wave functions found in the analysis of the exact shell model diagonalization [21] for the cases of smaller dimensions.

The classical derivation of the level density for given spin [2,3] is based on the idea of random coupling of individual particle spins into the total spin of the many-body system. This ''geometric chaoticity'' originates from the presence of many possible coupling schemes described by the complicated $3nj$ symbols rather than from specific features of nuclear forces. The random-walk process of spin coupling results in the Gaussian level density as a function of the total spin projection $J_z=M$,

$$\rho_M(E)=\frac{\rho(E)}{\sqrt{2\pi\sigma^2}}e^{-M^2/2\sigma^2}, \tag{2}$$

where $\rho(E)$ is the total density of states at excitation energy E, and σ^2 is the average value $\langle M^2\rangle$ in the shell model space. Assuming Eq. (2), the level density $\rho(E,J)$ for spin J can be obtained with no further approximations in a conventional way,

$$\rho(E,J)=\rho_{M=J}(E)-\rho_{M=J+1}(E), \tag{3}$$

which leads to the standard expression

$$\rho(E,J)=\frac{\rho(E)}{\sqrt{8\pi\sigma^3}}(2J+1)e^{-(J+1/2)^2/2\sigma^2}. \tag{4}$$

The next steps usually taken are the Fermi-gas approximation for the total density of states $\rho(E)$, the backward shift of the excitation energy, $E\rightarrow U=E-\Delta$, where $\Delta(Z,N)$ reflects the pairing threshold for two-quasiparticle excitations (in even-even nuclei), and the expression of σ in terms of the statistical (rigid body) moment of inertia.

One can notice that the random walk approximation (2)–(4) works much better for the total number of states, dimension $d(J)$ in Hilbert space, the quantity of a pure geometrical nature, than for the energy-dependent density $\rho(E,J)$ that is

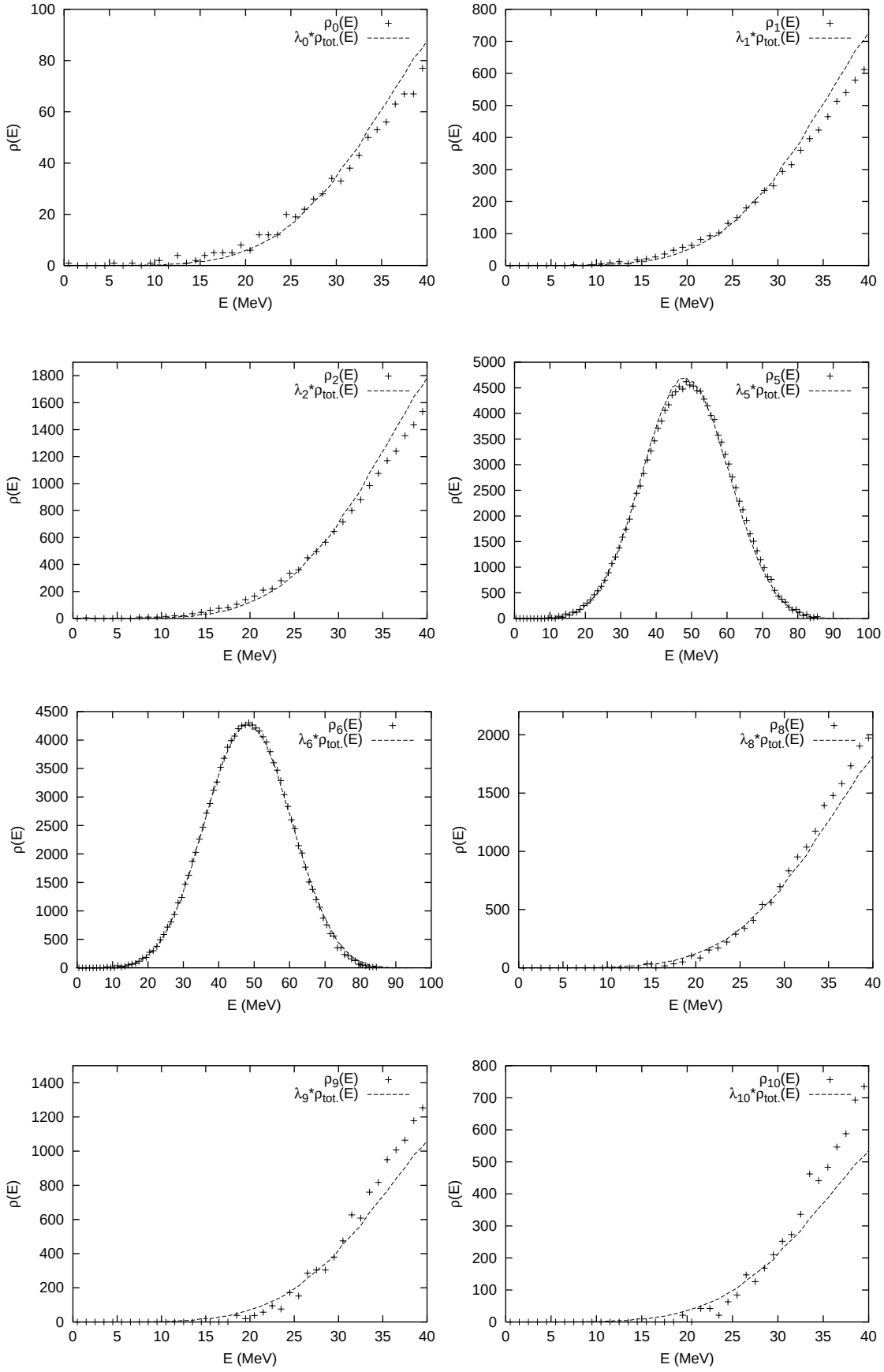

FIG. 2. Spin-dependent level densities $\rho(E,J)$ from shell model calculations (times $2J+1$) (crosses) and rescaled densities (broken lines) for 12 particles in the sd-shell.

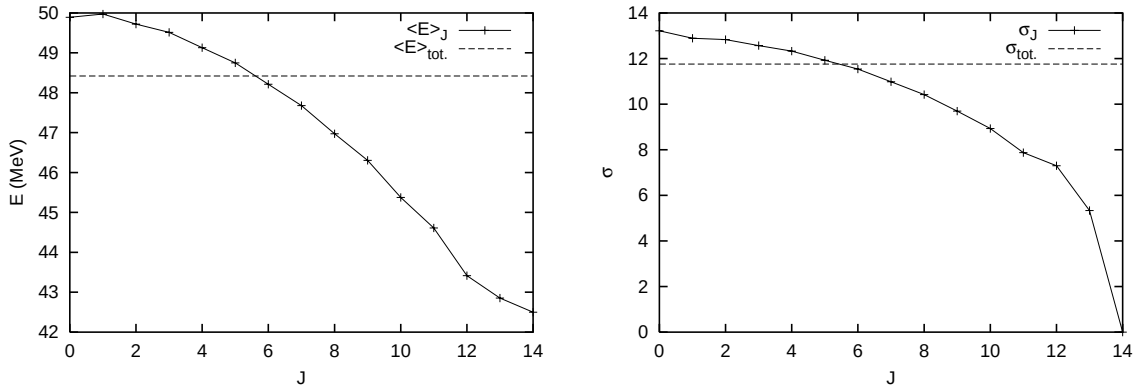

FIG. 3. Shell model scalar centroids and widths of the partial level density $\rho(E,J)$ as a function of total spin J for 12 particles in the sd-shell. Broken horizontal lines show the same quantities for the total density $\rho(E)$.

determined by the interaction dynamics. If one tries to rescale the partial level densities $\rho(E,J)$ from the total level density $\rho(E)$ of Eq. (1) with the aid of the scaling factors $\lambda_J = d(J)/d_{\rm tot}$, the deviations turn out to be much more pronounced (see Fig. 2), even for the most important low spins. The physical reason for this discrepancy is that the centroids and widths found according to the recipes of statistical spectroscopy [22,26] depend on spin, Fig. 3. Similar results for the J dependence of centroids and widths were reported in Refs. [31,32]. For $J=5$ and 6, the J-dependent scalar centroids and widths coincide with those of the total density (Fig. 3), and the rescaling scheme describes reasonably well the J-dependent level density, see Fig. 2. In fact, as a rule,

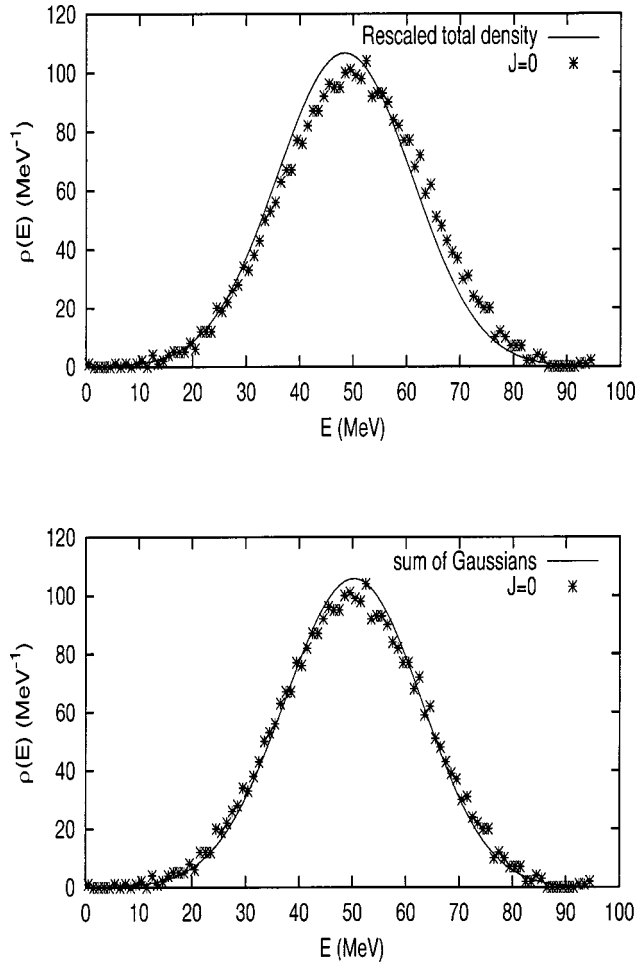

FIG. 4. $J=0$ shell model level density for 12 particles in the sd shell model (stars), compared with the rescaled total density $\lambda_0\rho(E)$ (upper panel), and fixed-J Gaussian sum of Eq. (9) (lower panel).

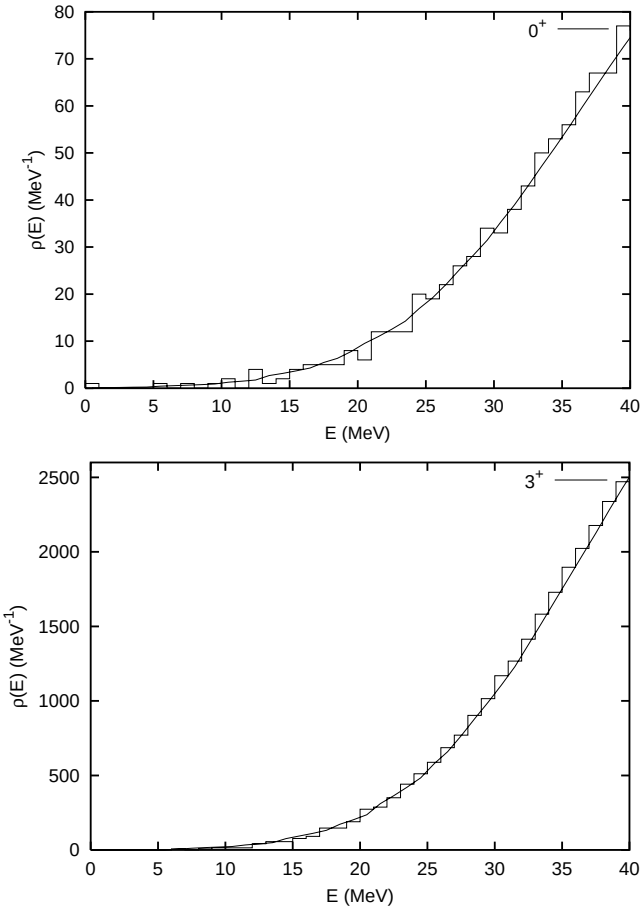

FIG. 5. Low energy part of $J=0$ (upper panel) and $J=3$ (lower panel) shell model level density times $2J+1$ for ^{28}Si (histogram) compared with the fixed-J sum of finite range Gaussians, Eq. (11).

the variance $\sigma_c(J)$ of the centroid distributions makes the main contribution to the total width $\sigma(J)$ larger than the average width of individual partitions weighted with their dimensions [22].

As a practical solution for the problem of calculation of shell-model level densities without full diagonalization we can suggest the following. For each shell model partition $p=1,\ldots,P$, the fixed-J centroid $\overline{E}_p(J)$ is calculated in accordance with the prescriptions of statistical spectroscopy [22,17], together with the fixed-J width $\sigma_p(J)$. Since the results for the level density obtained from the spectral moments are sensitive to the position E_0 of the ground state, we apply the method of exponential extrapolation to find the ground state energy. This method, based on the generic behavior of small admixtures of remote basis states to the wave functions of low-lying states, was suggested, tested, and justified by shell-model examples, random matrix theory, and exactly solvable models [25]. It was later successfully used for ground state energies of fp nuclei [37] and the superdeformed state in ^{56}Ni as well as for single-particle occupancies [33].

We remind the reader the main justification of the exponential extrapolation. The typical properties of complicated many-body states are revealed, for example, by a detailed analysis in the framework of the nuclear shell model [21]. Very similar results for complex atoms [20] show that these properties are indeed generic for many-body quantum chaos. It is practically important that the determination of the relevant global parameters does not require the diagonalization of the huge Hamiltonian matrix. The distribution of the components C_k^α of a many-body state $|\alpha\rangle$ in the basis of $J^\pi T$-projected independent particle configuration states $|k\rangle$ is close to the Gaussian predicted by the random matrix theory [1,18,19]. The same is valid for the strength functions

$$F_k(E)=\sum_\alpha |C_k^\alpha|^2 \delta(E-E_\alpha) \tag{5}$$

of the shell model basis states $|k\rangle$ for the realistic residual interaction strength [34]. The centroids $\overline{E}_k$ of these distributions are given by the diagonal matrix elements of the full Hamiltonian H,

$$\overline{E}_k \equiv \sum_\alpha |C_k^\alpha|^2 E_\alpha = H_{kk}. \tag{6}$$

The width σ_k of the strength function (5) is also known prior to the diagonalization as the sum of the off-diagonal matrix elements squared,

$$\sigma_k^2 \equiv \sum_\alpha |C_k^\alpha|^2 (E_\alpha^2 - \overline{E}_k^2) = \sum_{l(\neq k)} H_{kl}^2. \tag{7}$$

An illustration of these distributions for the case of $J^\pi T = 0^+0$ states of $A=12$ particles in the sd-shell model, where the USD interaction [27] was used, can be found in Figs. 1 and 2 of Ref. [35]. The results are qualitatively the same for different effective interactions; the fp-shell model provides also quite similar results. We need to stress that no diagonalization is required here. As was shown for the first time in Ref. [21], the widths σ_k are nearly constant, $\sigma_k \approx \overline{\sigma}$. The mechanism of this equilibration is provided by the above mentioned geometric chaoticity that is inevitably growing in the process of constructing $J^\pi T$-projected states [21,36]. As discussed earlier, the same chaoticity of almost random coupling of individual spins into total spin J is in the core of the standard derivation [1–3] of the spin-dependent level density. The fact of constancy of the widths σ_k is essential for establishing a practical boundary for the shell model truncation [35] on the level of $(3-4)\sigma$. This truncation gives a first approximation to the energy eigenvalues.

The further precise definition of energies of low-lying states can be achieved using the exponential extrapolation [25,37]. It was established [34] that the remote tails of the generic strength function are exponential. This can be translated into exponentially small admixtures of highly excited states, located beyond threshold of $(3-4)\sigma$ from the centroid, to the exact wave functions of low-lying states. The exponential convergence was rigorously proved in some models and tested by the full matrix diagonalization when possible. A practical algorithm was worked out [37] to establish the onset of the exponential regime by several progressive truncations keeping the partitions in their entirety. Using this algorithm, it is usually possible to locate the ground and low-lying states very close (better than 200–300 keV) to the exact energy value using shell model spaces of dimensions that are less than 1% of the full dimension [37,33].

With the knowledge of the ground state position we determine the set of the Gaussians,

$$G_p(E,J) \equiv G[E+E_0-\overline{E}_p(J), \sigma_p(J)], \tag{8}$$

where E is the excitation energy from the ground state of energy E_0. The superposition of the contributions of the partitions weighted with their dimensions $d_p(J)$ leads to the full level density

$$\rho(E,J)=\sum_p^P d_p(J) G_p(E,J). \tag{9}$$

In this approach each partition has a definite number of particles and parity; no special effort for conserving number of particles and parity is required, as in the case of a model that cannot select subspaces with correct symmetries, such as shell model Monte Carlo [38,39]. The generalization to the fixed-isospin level density is straightforward. $\overline{E}_p(J)$ and $\sigma_p(J)$ are calculated using techniques similar to those described in Ref. [22].

A part of the present approach was sometimes mentioned in the literature as a method to determine the shape, but not the J-dependent level density $\rho(E,J)$. A novel feature here is the opportunity of estimating the position of the ground state with very good accuracy [25,37]; the method works if the ground state energy is known with an accuracy not worse than 100–200 keV. But this is the precision one can achieve with the aid of the exponential convergence [37]. The exponential convergence method was recently proven to work for many major shells, and many $\hbar\omega$ excitations [40]. Figure 4

shows the results for this approach applied to the case of 12 valence particles in the *sd*-shell model using the USD interaction of Ref. [27].

Recently, a method proposed by Zuker [23], which uses four scalar moments, was generalized by Johnson and collaborators to the sum of configurations [41–43]. Due to the complexity of the calculations, they could not obtain all *J*-dependent moments, as in Eq. (9). Therefore, they relied on a rescaling procedure based on Eq. (4), but using an energy dependent spin-cutoff factor σ. This approach attempts to calculate more accurately the shape of the total density of states, but introduces two new approximations, Eq. (4) and the approximate calculation of $\langle \hat{J}^2 \rangle(E)$, that could affect the overall accuracy. Figs. 2–4 of Ref. [43] do not prove that the inclusion of the third and fourth moments improves the accuracy of the results.

One can understand why our sum using only the first and second moments, Eq. (9), turns out to be so reliable. Although the higher moments describing skewness and excess are significant, in adding contributions from many configurations, the asymmetries have a tendency to average out. As Fig. 1 of Ref. [35] suggests, the only configurations for which the asymmetry may survive are those with the centroids close to the edges of the spectrum. In addition, the ranges of those distributions are finite [typically, the ranges of the spectrum are about $(12–16)\sigma$]. To take into account these effects, we replaced the Gaussians in Eq. (9) by the finite range Gaussians (FRGs) that span over a range of at most $\pm 3\sigma$, and do not extend lower than the energy of the yrast state for each spin,

$$G_p(E,J) \mapsto (\mathrm{FRG})_p(E,J,E_J), \tag{10}$$

where

$$(\mathrm{FRG})_p(E,J,E_J) = \sqrt{\frac{2}{\pi}} \frac{e^{-t^2}}{\sigma[\mathrm{erf}(t_-)+\mathrm{erf}(t_+)]} \tag{11}$$

if $t_- < t < t_+$, and 0 otherwise. Here

$$t = \frac{E + E_0 - \overline{E}_p(J)}{\sqrt{2}\sigma}, \tag{12}$$

t_- corresponds to either the $\overline{E}_p(J) - 3\sigma$ or the yrast state energy (whichever is higher), and, similarly, $t_+ = \overline{E}_p(J) + 3\sigma$. The choice of $\pm 3\sigma$ for the FRGs is based on the observation of Ref. [35] (see, e.g., Fig. 3 of Ref. [35]) that, for the low-lying states, the configurations located within $\pm 3\sigma$ to the centroid provide more than 90% of the overlap with the exact wave function. An accurate calculation of the yrast state energy can be obtained using the exponential convergence method with the same effort as for the ground state energy [25,37].

The results obtained with the use of this procedure are shown in Fig. 5 for the lowest part of spectrum in the cases of $J=0$ and $J=3$. Figure 6 shows the density of 0^+ and 0^- states for six particles in *psd* model space using the PSDMK interaction [44] (no attempt was made to remove the center-of-mass spurious components; the effect of the center-of-mass spurious motion on the nuclear level density is still under investigation [43,48]). The comparison with exact shell model calculations proves to be very good.

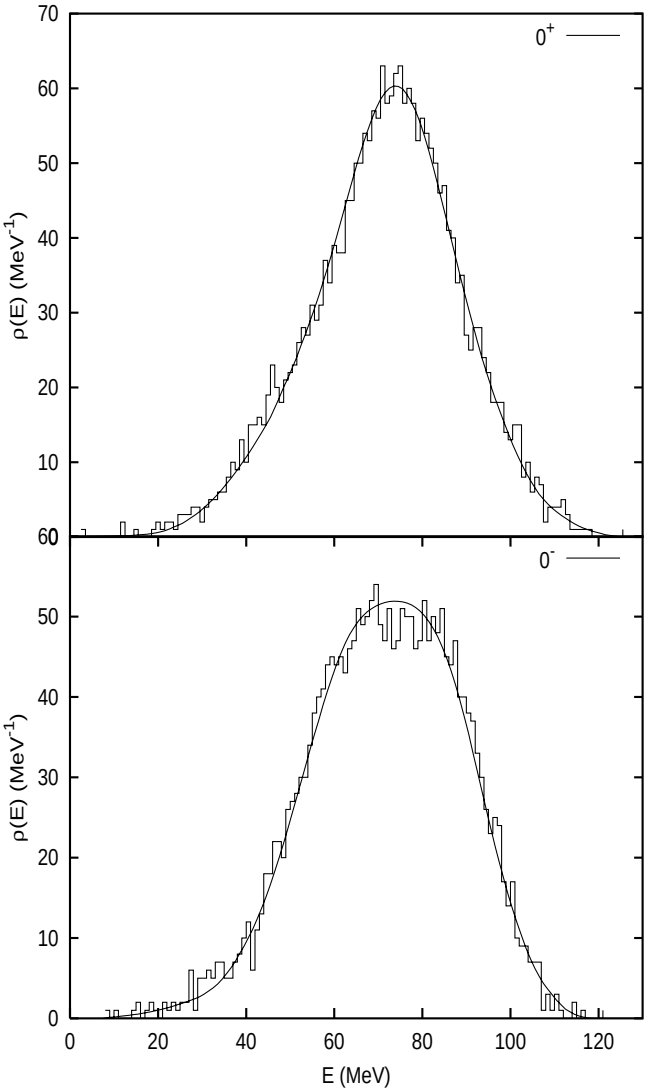

FIG. 6. $J=0$ shell model level density for 6 particles in *psd* model space (histograms) compared with the fixed-*J* sum of finite range Gaussians, Eq. (11); upper panel shows the density of positive parity states, while lower panel shows the negative parity states.

In conclusion, we proposed a new practical method of calculating the total density of states using the procedure of statistical spectroscopy for the centroids and widths for each partition in a given shell model space. We show that the rescaling scheme based on Eq. (4) for the total density of states, sometimes used with the Fermi-gas and Monte Carlo methods [28], is not accurate enough in describing shell model *J*-dependent densities, especially for low spins *J* that are of special interest in applications. However, a sum of Gaussians over partitions with the *J*-dependent centroids and widths, Eqs. (8)–(12), can successfully describe spin- and parity-dependent partial level densities; the essential ingredient is an accurate estimate of the ground state energy of the system, which is possible with the aid of the exponential convergence method.

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