Statistical spectroscopic calculation of expectation values and spin-cutoff factors

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Abstract

Recently we proposed a formalism, based in nuclear statistical spectroscopy, for efficient computation of nuclear level density, or densities of states, through a sum of partitioned binomial functions (SUPARB). In this Letter we extend the formalism to the calculation of locally averaged expectation values, with specific application to spin-cutoff factors and the angular momentum dependence of the nuclear density of states.
In a recent Letter [1] we proposed a computationally efficient method to compute nuclear level densities, based in the ideas of nuclear statistical spectroscopy [2–4]. While we refer interested readers to our original Letter for details, we briefly summarize here. Consider the density of states of a Hamiltonian $\hat{H}$,

$$\rho(E) = \text{tr} \delta(E - \hat{H}).$$  \hspace{1cm} (1)

It is useful to partition the finite model space into subspaces, labeled by Greek letters $\alpha, \beta$, etc., each with an associated projection operator $P_\alpha$. Then one can define partial or configuration densities:

$$\rho_\alpha(E) = \text{tr} P_\alpha \delta(E - \hat{H}).$$  \hspace{1cm} (2)

The total density is the sum of the partial densities. (NB:We always include $2J + 1$ degeneracies and so are formally considering state densities.)

If the subspaces are single-particle configurations, e.g., $(0d_{5/2})^4, (0d_{5/2})^2(1s_{1/2})^2$, etc, then the partial, or configuration, moments up to fourth order for any system with $Z$ protons and $N$ neutrons in the valence space can be computed directly from the one+two-body matrix elements of $\hat{H}$ [5,6]. For any partition (configuration) $\alpha$ let $d_\alpha = \text{tr} P_\alpha$ be the dimension of the subspace $\alpha$, and define the configuration average over the subspace to be $\langle \ldots \rangle_\alpha \equiv d_\alpha^{-1} \text{tr} P_\alpha(\ldots)$. Then $\bar{E}(\alpha) = \langle \hat{H} \rangle_\alpha$ is the (configuration) centroid, $\gamma(\alpha) = \langle (\hat{H} - \bar{E}_\alpha)^2 \rangle_\alpha^{1/2}$ the configuration width, $m_3(\alpha) = \langle (\hat{H} - \bar{E}_\alpha)^3 \rangle_\alpha / \gamma^3(\alpha)$ the scaled (dimensionless) third configuration moment, and $m_4(\alpha) = \langle (\hat{H} - \bar{E}_\alpha)^4 \rangle_\alpha / \gamma^4(\alpha)$ the scaled fourth configuration moment.

With these moments in hand, we model the partial densities as binomial distributions, following a recent suggestion of Zuker [7]. Starting with the binomial expansion of $(1 + \lambda)^N$ and representing $\binom{N}{k}$ with gamma functions, one can derives a continuous distribution,

$$\rho(E_x) = \lambda^{E_x/\epsilon} \frac{\Gamma(E_{\text{max}}/\epsilon + 1)}{\Gamma(E_x/\epsilon + 1)\Gamma((E_{\text{max}} - E_x)/\epsilon + 1)}$$  \hspace{1cm} (3)

where $E_x$ is the excitation energy and $E_{\text{max}} = \gamma(1 + \lambda)\sqrt{N/\lambda}$ is the maximum excitation energy in the binomial distribution. The binomial is appealing because one can easily
compute the scaled third and fourth central moments: $m_3 = \frac{1}{\sqrt{N\lambda}}$ and $m_4 = 3 - \frac{4\lambda}{N} + \frac{1}{N\lambda}$, allowing one to control the shape of the binomial through $N$ and $\lambda$.

To compute the density of states, we take the following steps: (1) We compute the configuration moments up to 3rd or 4th order. (2) We model the partial density for each configuration as a binomial. The binomial parameters $N$ and $\lambda$, as well as the overall energy scale and centroid, are fitted to the configuration moments. (3) The partial densities are summed to yield the total density of states. Because of these ingredients, we will refer to our approach as SUPARB (SUm of PARtitioned Binomials) state densities. We have shown that our method models well the density of states, when compared against exact calculations, and that one needs third configuration moments and occasionally, but not always, fourth configuration moments to achieve accurate results [1]. Incidentally, none of this is special to the atomic nucleus. One could easily apply it to atomic electrons as well.

We now turn to the computation of expectation values of some general operators, $\hat{O}$, and define the energy-dependent locally averaged expectation value (LEV) as

$$\langle \hat{O}(E) \rangle = \frac{\text{tr} \hat{O} \delta(E - \hat{H})}{\text{tr} \delta(E - \hat{H})}. \quad (4)$$

We also have configuration LEVs:

$$\langle \hat{O}(E) \rangle_\alpha = \frac{\text{tr} P_\alpha \hat{O} \delta(E - \hat{H})}{\text{tr} P_\alpha \delta(E - \hat{H})}. \quad (5)$$

Our strategy for computing the total $\langle \hat{O}(E) \rangle$ is the same as for the total density of states. In addition to the configuration moments, we compute the weighted averages $\langle \hat{O} \rangle_\alpha$, $\langle \hat{O}(\hat{H} - \bar{E}_\alpha) \rangle_\alpha$, and $\langle \hat{O}(\hat{H} - \bar{E}_\alpha)^2 \rangle_\alpha$. These can be computed directly from one+two-body matrix elements similar to those for the moments [5,6].

The only tricky point is if $\hat{O}$ and $\hat{H}$ do not commute; where does one insert the projection operator $P_\alpha$ in eqn. (5)? Because $\sum_\alpha P_\alpha = 1$ by the completeness of the projection operators, we conclude consistency is the only requirement, and take $\text{tr} P_\alpha \hat{O} \hat{H}^k$, $k = 0, 1, 2$.

Assume within any subspace a quadratic energy dependence, that is,

$$\langle \hat{O}(E) \rangle = O_0 + O_1(E - \bar{E})/\gamma + O_2(E - \bar{E})^2/\gamma^2 \quad (6)$$

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(dropping for the moment the subspace label $\alpha$). Then

$$\langle \hat{O} \rangle = O_0 + O_2,$$  \hspace{1cm} (7)

$$\langle \hat{O}(\hat{H} - \bar{E}) \rangle = \gamma(O_1 + O_2 m_3),$$  \hspace{1cm} (8)

$$\langle \hat{O}(\hat{H} - \bar{E})^2 \rangle = \gamma^2(O_0 + O_1 m_3 + O_2 m_4).$$  \hspace{1cm} (9)

Solving for coefficients,

$$O_0 = \frac{\langle \hat{O}\rangle (m_4 - m_3^2) + m_3 \langle \hat{O}(\hat{H} - \bar{E})\rangle / \gamma - \langle \hat{O}(\hat{H} - \bar{E})^2\rangle / \gamma^2}{m_4 - m_3^2 - 1},$$  \hspace{1cm} (10)

$$O_1 = \frac{(m_4 - 1) \langle \hat{O}(\hat{H} - \bar{E})\rangle / \gamma + m_3 \left( \langle \hat{O}(\hat{H} - \bar{E})^2\rangle / \gamma^2 - \langle \hat{O} \rangle \right)}{m_4 - m_3^2 - 1},$$  \hspace{1cm} (11)

$$O_2 = \frac{\langle \hat{O}(\hat{H} - \bar{E})^2\rangle / \gamma^2 - m_3 \langle \hat{O}(\hat{H} - \bar{E})\rangle / \gamma - \langle \hat{O} \rangle}{m_4 - m_3^2 - 1}.$$  \hspace{1cm} (12)

If we limit ourselves to only a linear dependence (assume $O_2 = 0$), then

$$O_0 = \langle \hat{O}\rangle,$$  \hspace{1cm} (13)

$$O_1 = \langle \hat{O}(\hat{H} - \bar{E})\rangle / \gamma.$$  \hspace{1cm} (14)

Note: in terms of the binomial parameters $N, \lambda$, one finds that $m_4 - m_3^2 - 1 = 2(1 - N^{-1})$.

The generalization to the full SUPARB case, summing over partitions, is easy:

$$\langle \hat{O}(E) \rangle = \sum_\alpha \frac{\langle \hat{O}(E) \rangle_\alpha \rho_\alpha(E)}{\rho(E)}.$$  \hspace{1cm} (15)

In Figures 1-3 we illustrate our method, comparing to “exact” shell model calculations in full $0h\omega$ spaces. For $sd$-shell nuclides we used the Wildenthal USD interaction [8], and compared against direct diagonalization. Fig. 1 shows the LEV of $\vec{Q} \cdot \vec{Q}$ and $S^2$ for $^{20}\text{Ne}$, while Fig. 2 shows the LEV of $J^2$ (which will be important for the spin-cutoff factor below) for $^{22}\text{Na}, ^{23}\text{Mg}$, and $^{32}\text{S}$.

Fig. 3 compares the LEV of $J^2$ for $^{48}\text{Cr}$ and $^{54}\text{Fe}$ in a full $0h\omega pf$-shell calculation; here the “exact” calculation was through Monte Carlo sampling of path integrals [4][10]. To avoid the well-known sign problem [11] we fitted a schematic multipole-multipole interaction to the $T = 1$ matrix elements of the FPD6 interaction of Richter et al. [12]. Clearly the full
SUPARB calculation, with a quadratic dependence in each partition, works very well, and
the quadratic is a significant improvement over the linear approximation. One could go to
a cubic dependence, but computation of the necessary moments, while possible, would be
very time consuming and there is not much room for improvement.

Now we apply our formalism to spin-cutoff factors for state densities. Define the $J$-
dependent density as

$$\rho(E, J) = \text{tr} \left( \delta(E - \hat{H})\delta(J(J + 1) - \hat{J}^2) \right).$$

(16)

Traditionally this is factorized to

$$\rho(E, J) = \rho(E)(2J + 1)\Omega(J, E),$$

(17)

and one assumes a weighted Gaussian form for $\Omega$:

$$\Omega(J, E) = (2J + 1) \frac{1}{4\sigma(E)\sqrt{2\pi}} \exp \left( -\frac{(J + \frac{1}{2})^2}{2\sigma(E)^2} \right)$$

(18)

We have normalized $\int dJ\Omega(J, E) = 1$. Here $\sigma(E)$ is the “spin-cutoff” factor and is dependent
on the energy. The spin-cutoff factor has been considered before in the context of nuclear
statistical spectroscopy [13], but the moments were computed by a random sampling of
representative vectors and the level densities were approximated by Hermite polynomials
(which do not guarantee nonnegative densities).

Given the form (18) one finds that

$$\langle \hat{J}^2 \rangle = 3\sigma^2 - \frac{1}{4}$$

(19)

(The factor of 3 is because we must include the $2J + 1$ degeneracy in our traces.) Therefore,
the problem of describing $\rho(E, J)$ with SUPARB reduces to computing $\langle \hat{J}^2 \rangle$ as a function
of energy, which were given in figures 2 and 3.

In figure 4 we plot the exact and SUPARB $J$-projected level densities (without the $2J + 1$
degeneracy) of $^{32}$S, for $J = 0, 1, 2$ and 8. The results are very good. Incidentally, one could
compute the spin-cutoff factors and thus the $J$-projected level densities using Monte Carlo
evaluation of path integrals just as easily, although this has not yet been done.
In summary, we have extended our previous SUPARB technique for state densities to expectation values of operators, including application to spin-cutoff factors. Our results look very good. Other possible application include estimating the contamination of spurious states in cross-shell calculations, and computation of total strengths and energy-weighted sum rules for transitions.

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FIG. 1. Comparison of exact shell model locally-averaged expectation value of (a) $\vec{Q} \cdot \vec{Q}$ and (b) $S^2$ in $^{20}$Ne. The histogram is from direct diagonalization, and we compare against both linear (dashed line) and quadratic (solid line) SUPARB estimates.

FIG. 2. Comparison of exact shell model locally-averaged expectation value of $J^2$ in (a) $^{22}$Na, (b) $^{23}$Mg, and (c) $^{32}$S. The circles are from direct diagonalization, and we compare against both linear (dashed line) and quadratic (solid line) SUPARB estimates.
FIG. 3. Comparison of exact shell model locally-averaged expectation value of $J^2$ in (a) $^{48}$Cr, and (b) $^{54}$Fe. The histogram is from Monte Carlo sampling of a path integral, and we compared against both linear (dashed line) and quadratic SUPARB (solid line) estimates.

FIG. 4. Comparison of $J$-projected state densities in $^{32}$S for $J = 0, 1, 2,$ and $8$. The circles are ‘exact’ from direct diagonalization, and the solid lines are SUPARB estimates with spin-cutoff factor.