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Spectral distribution theory—Some recent applications

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Abstract. The application of spectral distribution theory for binding energy, spectra and occupancies using universal-*sd* interaction in (*sd*) shell and for Gamow-Teller and M1 strength sums in both (*fp*) and (*sd*)-shell is described.

Keywords. Spectral distribution theory; binding energy; Gamow-Teller strength.

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1. Introduction

Spectral distribution theory describes different aspects of nuclear spectra and excitation strengths in a statistical framework. This theory has been successful in developing many physical principles as well as formal results for treating nuclear spectra, transition strengths and sum rules for nuclear excitations, fluctuations in spectra and strengths, etc. The application of these results to specific nuclei and comparison of the theoretical predictions with experimental quantities or with the predictions of shell model and other theories, are important and need sustained efforts. In this paper we review some recent studies on the application of spectral distributions to nuclei in the (*sd*) as well as the (*fp*) shell.

2. Spectral distribution theory

We briefly describe some important results of spectral distribution theory. The density of energy eigenstates in large many-nucleonic spaces tends to a gaussian (or a sum of gaussians) asymptotic form. This result is derived by calculating the moments of the hamiltonian using random matrix forms for the 2-body hamiltonian and using the central limit theorem (CLT) (Mon and French 1975). For specific interactions in (*sd*) and (*fp*) shell, numerous shell model calculations have shown that in large spaces with not too few nucleons, the departure from the asymptotic result as measured by third and higher order cumulants is small. The effect of the small skewness and excess (γ_1 and γ_2) can also be incorporated in the theory. The asymptotic gaussian form for the density is seen to be valid even in specific configuration and isospin-partitioned spaces (denoted by $\mathbf{m}$, T).

The ground state energy (E_g) of a nucleus with degeneracy d_0 is calculated in spectral distributions by inverting the equation for the intensity $I_{\mathbf{m},T}(E)$ (the density of states

normalized to give the total dimensionality of the space)

$$\sum_{\mathbf{m}} \int_{-\infty}^{E_g} I_{\mathbf{m},T}(E)\,\mathrm{d}E = d_0/2. \tag{1}$$

This procedure due to Ratcliff (1971) is improved by integrating up to an excited state energy and then subtracting the experimentally observed excitation energy from it. The correction of the ground state energy due to non-zero (γ_1, γ_2) is obtained by utilizing the Cornish-Fisher expansion (Kota *et al* 1986).

The expectation value of any operator K in a state with energy E is given by a polynomial expansion in E as

$$\langle E|K|E\rangle = K(E) = \frac{d(m)}{I_m(E)} \langle K\delta(H-E)\rangle^m = \sum_\nu \langle KP_\nu(H)\rangle^m P_\nu(E), \tag{2}$$

where $d(m)$ and $I_m(E)$ are the dimensionality and the intensity at energy E in the m-particle space and $\langle\ \ \rangle^m$ denotes averages $(=\text{traces}/d(m))$ in the m particle space. $P_\nu(x)$ are the orthonormal polynomials with the density $\rho_m(E)$ $(=I_m(E)/d(m))$ as the weight function. For example $P_0(x) = 1$ and $P_1(x) = (x-\varepsilon_x)/\sigma_x$, where ε_x and σ_x are the centroid and the width of the variable x. The distribution theory gives a nice geometrical structure to the operators in terms of the norm, defined by $\|A\| = \langle A^\dagger A\rangle^m$ for the operator A and the correlation coefficient between two operators, defined by $\zeta_{AB} = \langle (A-\langle A\rangle^m)(B-\langle B\rangle^m)\rangle^m/\sigma_A\sigma_B$ for operators A and B, where σ_A and σ_B are the widths of operators A and B $[\sigma_A^2 = \langle A^2\rangle^m - (\langle A\rangle^m)^2]$. Assuming the density of states for the hamiltonian H as well as for the perturbed hamiltonian $H_\alpha = H + \alpha K$ to be gaussians one gets the CLT result

$$K(E) \xrightarrow{\text{CLT}} \langle K\rangle^m + \left\langle K\frac{(H-\varepsilon)}{\sigma}\right\rangle^m \frac{(E-\varepsilon)}{\sigma} = \langle K\rangle^m + \zeta_{K-H}\sigma_K(E-\varepsilon)/\sigma$$
$$= K_0(E) + K_1(E) = K_{\text{CLT}}(E). \tag{3}$$

This linear form has a straightforward extension to configuration isospin spaces.

For any excitation operator O, the non-energy weighted (NEW) sum rule for excitation from the state with energy E is obtained by taking $K = \mathrm{O}^+\mathrm{O}$ in (2). For the ground state $(E_g - \varepsilon)/\sigma < 0 (\sim -3{\cdot}5)$ and thus the sum rule strength in the ground state region is small when ζ_{K-H} is positive and large whereas the sum rule strength in the ground state region is large when ζ_{K-H} has large negative values. On the other hand for $\zeta_{K-H} \sim 0$, $K(E)$ is approximated quite well by just its average value $\langle K\rangle^m$.

The question one can naturally ask at this stage is under what conditions the density of H and that of $H + \alpha K$ remain the same and how does one take account of the departures from this result. Questions like these are not yet very well studied and need careful attention. One obvious way to study the departures is to go beyond the CLT limit expression. The next term in the expansion beyond CLT in (2) is given by $K_2(E) = \langle KP_2(H)\rangle^m P_2(E)$ and using $P_2(x) = (\hat{x}^2 - \gamma_1\hat{x} - 1)/(\gamma_2 + 2 - \gamma_1^2)^{\frac{1}{2}} \xrightarrow{\gamma_1=\gamma_2=0}$, $(\hat{x}^2-1)/\sqrt{2}$ where $\hat{x}$ is the standardized variable $(\hat{x} = (x-\varepsilon_x)/\sigma_x)$ this becomes

$$K_2(E) = \tfrac{1}{2}\langle K\{(\hat{H})^2 - 1\}\rangle^m (\hat{E}^2 - 1). \tag{4}$$

To find the relative importance of this term compared to $K_1(E)$ one can use the following criterion

$$\eta(E) = \frac{|K_2(E)|}{|K_1(E)|} = \frac{\zeta_{K-H-H}}{2\zeta_{K-H}} \left| \hat{E} - \frac{1}{\hat{E}} \right| \ll 1, \tag{5}$$

where

$$\eta_{K-H-H} = \langle (K - \langle K \rangle)(H - \varepsilon)^2 \rangle^m / \sigma_K \sigma^2.$$

It is easy to see that $\eta_{K-H-H} \leqslant \eta_{K-H}$. As in the ground state domain $\hat{E} \sim -3{\cdot}5$, the contribution from $K_2(E)$ is small when $K_1(E)$ itself is small (i.e. $\zeta_{K-H} \sim 0$). In §3, we shall see examples of these for specific excitation operators.

Spectral distribution theory also predicts expansions for the transition strength $R(E, E')$ from state $|mE\rangle$ with m particles and energy E to state $|m'E'\rangle$ with m' particles and energy E' defined as $R(E, E') = |\langle m'E'|O|mE\rangle|^2$. A formal expansion, using the polynomial defined by $\rho(E)$, can be derived for $R(E, E')$. This is given by

$$R(E, E') = \frac{1}{\mathrm{d}(m')} \sum_{\mu,\nu} \langle O^\dagger P'_\mu(H) O P_\nu(H) \rangle^m P'_\mu(E') P_\nu(E). \tag{6}$$

However the convergence properties of this expansion are, as yet, not well understood (French *et al* 1987a, b 1988). In a similar fashion one can develop smoothed CLT forms for the strength density defined by

$$S(E, E') = I_m(E) I_{m'}(E') \frac{R(E, E')}{\mathrm{d}(m) \langle O^\dagger O \rangle^m}.$$

This way one can also develop asymptotic forms for the non-energy weighted sum rule strength density and this suggests a promising way of evaluating sum rule quantities. For detailed discussions on these we refer to French *et al* (1987a, b, 1988). For other important results and discussions on this subject we refer to a few reviews on the subject (French 1980; French and Kota 1982; Kota and Kar 1988).

3. Applications

3.1. *Binding energies, spectra and occupancies in (sd)-shell with Wildenthal's universal-sd interaction*

In testing the predictions of the spectral distribution theory, one inherent uncertainty lies in the choice of the interaction. Recent shell model calculations in the (*sd*)-shell however showed phenomenal success of A-dependent (two-body matrix elements taken to be proportional to $(18/A)^{0{\cdot}3}$) interaction proposed by Wildenthal, in reproducing binding energies, spectra, spectroscopic factors and transition strengths of electromagnetic and beta excitations (Wildenthal 1984). This universal-*sd* interaction seems to be the interaction to use for calculations throughout the (*sd*)-shell and we recently carried out spectral distribution calculations with this (Sarkar *et al* 1987). In figure 1 we show a comparison of the predictions of binding energies with the experimental values (the shell model values are always within 200 keV of the experimental ones). The figure also demonstrates how strikingly the (γ_1, γ_2) corrections improve the predictions. The low energy excitation spectra have also been

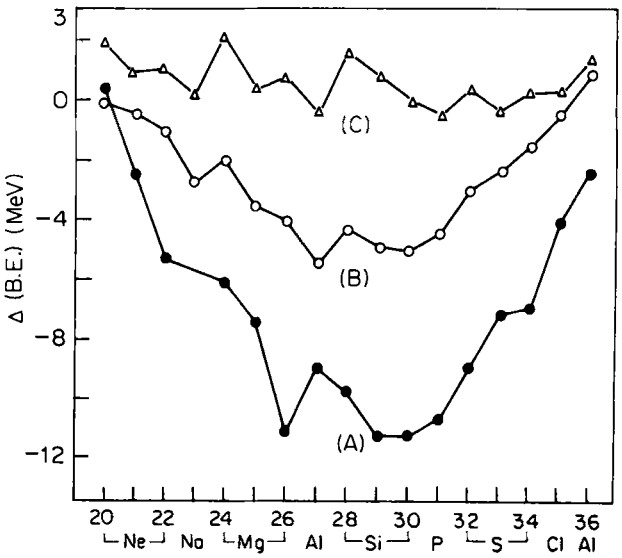

Figure 1. Comparison of binding energy (B.E.) predictions (Sarkar *et al* 1987) by spectral distributions (SDM) with experimental values. Figure shows $\Delta(\text{B.E.}) = (\text{B.E.})_{\text{SDM}} - (\text{B.E.})_{\text{exp}}$ curve A stands for results without any corrections, curve B with excited state and curve C with excited state and (γ_1, γ_2) corrections (taken from Kota and Kar 1988).

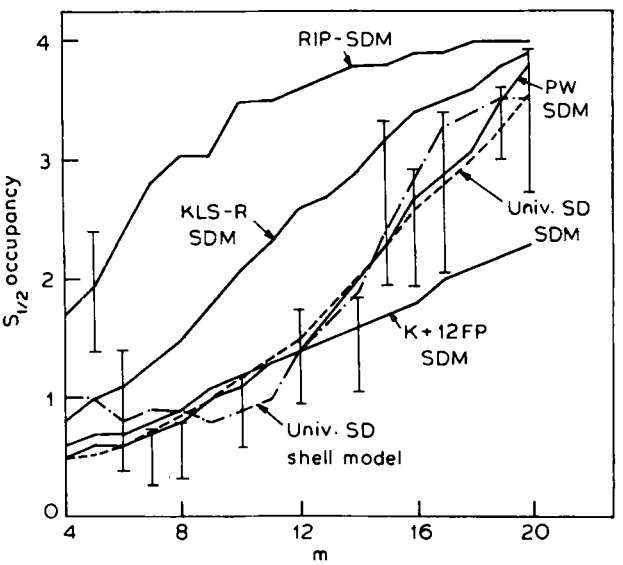

Figure 2. $S_{1/2}$ ground state occupancies by spectral distribution methods (SDM) using universal-*sd*, PW, RIP, KLS-R and K + 12FP interactions compared with experimental values. The results for PW, RIP, K + 12FP and KLS-R interactions, and the experimental data are from Potbhare and Pandya (1976). The results for universal-*sd* interaction are from Sarkar *et al* (1987).

compared. Also the calculation of occupancies of the $d_{5/2}$, $d_{3/2}$ and $s_{1/2}$ orbits shows good agreement with shell model except for the $d_{3/2}$ orbit in the lower half of the shell. Figure 2 shows a comparison of $s_{1/2}$ occupancy with experimental numbers obtained

from stripping and pickup data. It includes predictions using other interaction also (Potbhare and Pandya 1976) and universal-*sd* along with PW clearly seems to be the best.

3.2 *Gamow-Teller and M1 sum rules and strength distributions*

Sum rules for Gamow-Teller (GT) strengths in the (*sd*) and (*fp*) shell is important to study the question of quenching. The most widely used sum rule involves the total β^- and β^+ strengths, S_{β^-} and S_{β^+} of the same nucleus (N, Z) and is given by

$$S_{\beta^-} - S_{\beta^+} = 3(N - Z). \tag{7}$$

But this is useful to evaluate S_{β^-} for nuclei with closed proton shells (^{48}Ca, ^{90}Zr etc) where $S_{\beta^+} = 0$. The Gamow-Teller operator is given by $O_{\mathrm{GT}} = \sum_i \boldsymbol{\sigma}(i)\mathbf{t}(i)$ where $\mathbf{t} = \frac{1}{2}\boldsymbol{\tau}$, $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ being the Pauli matrices in the spin and isospin spaces. In (*sd*)-shell the sum rules can be calculated by present versions of the shell model for all nuclei throughout, though in the middle of the shell it involves diagonalization of huge matrices. Hino *et al* (1987, 1988) evaluated the ground state GT and M1 strength sum by calculating the expectation value O^+O in the shell model ground state. In (*fp*)-shell the few shell model calculations performed to date (Bloom and Fuller 1985; Sekine *et al* 1987) use, by necessity, truncated spaces. Separate sum rules for β^- and β^+ strengths in the ground state have also been formulated (Sarkar and Kar 1985; Mac-Farlane 1986) for even-even nuclei but with the assumption that protons and neutrons in the ground state couple to zero-spin separately. These sum rules are

$$\begin{aligned} S_{\beta^-} &= 3 \sum_{nljj'} |C_{nl}^{jj'}|^2 \{1 - \langle n_{nlj}^P \rangle\} \langle n_{nlj'}^N \rangle, \\ S_{\beta^+} &= 3 \sum_{nljj'} |C_{nl}^{jj'}|^2 \{1 - \langle n_{nlj}^N \rangle\} \langle n_{nlj'}^P \rangle. \end{aligned} \tag{8}$$

with

$$C_{nl}^{jj'} = \{2(2j+1)(2j'+1)\}^{1/2} W(l\tfrac{1}{2}j1; j'\tfrac{1}{2}),$$

where n_{nlj}^P and $n_{nlj'}^N$ are fractional proton and neutron occupancies in orbits (nlj) and (nlj') respectively.

Spectral distributions have been successfully used for the evaluation of the GT as well as the $\mathrm{M1}^{\Delta T=1}$ sum rules and these methods give a geometrical understanding of why the expressions of (8) are successful in (*fp*)-shell but fail in (*sd*).

3.2(i) *GT strength sums in (fp)-shell–case with small correlation coefficient*: The correlation coefficient of $K = O_{GT}^+ O_{GT}$ with the hamiltonian (using the MHW2 interaction (McGrory *et al* 1970)) for self-conjugate nuclei (i.e. for nuclei with $N = Z$ or ground state $T = 0$) in (*fp*)-shell is seen to vary from 0·015 to 0·02. Thus the ground state Gamow-Teller strength sum ($S_{\beta^-} = S_{\beta^+}$ in this case) with only the first term in the expansion is calculated to be 9·6, 12·6 and 14·4 for the nuclei ^{48}Cr, ^{52}Fe and ^{56}Ni whereas keeping terms upto CLT makes them 9·2, 12·0 and 13·6 (Sarkar and Kar 1988a). Thus the contribution of the second term in (3) is seen to be small and retaining only the first term is not a bad approximation. This immediately explains why the expressions for S_{β^-} and S_{β^+} in (8) should work well in (*fp*)-shell. If one converts the operators and the states to proton-neutron formalism, the first term of (2)

is exactly the same as the expressions of (8). To see this we write for β^- decay

$$O_{\mathrm{GT}} = \sum_{r,s} \varepsilon_{rs}(pn)((a_p^\dagger)^{rj} \times a_n^{sj})^1 \tag{9}$$

where $(a_p^\dagger)^{rj}$ and a_n^{sj} are the proton creation and neutron annihilation operators in the orbits denoted by $r(nlj)$ and $s(nlj')$ and $\varepsilon_{rs}^1(pn)$ is the matrix element of the Gamow-Teller β^--decay operator in p-n language and given by

$$\varepsilon_{rs}^1(pn) = \varepsilon_{rs}^1(np) = C_{nl}^{jj'} = [2(2j+1)(2j'+1)]^{\frac{1}{2}} W(l\tfrac{1}{2}jl;j'\tfrac{1}{2}).$$

Then the non-energy weighted sum rule (NEWSR) operator becomes

$$\begin{aligned} O_{\mathrm{GT}}^\dagger O_{\mathrm{GT}} &= -\sqrt{3} \sum_{rstu} \varepsilon_{tu}^1(np)\varepsilon_{sr}^1(pn)[((a_n^\dagger)^{tj} \times a_p^{uj})^1 \times ((a_p^\dagger)^{sj} \times a_n^{rj})^1]^0 \\ &= -\sqrt{3} \sum_{rstu} \varepsilon_{tu}^1(np)\varepsilon_{sr}^1(pn) U(t_j u_j r_j s_j; 10) \\ &\quad \times [((a_n^\dagger)^{tj} \times a_n^{rj})^\nu \times (a_p^{uj} \times (a_p^\dagger)^{sj})^\nu]^0. \end{aligned} \tag{10}$$

If we consider an expansion like in (2) of the sum rule operator in the proton-neutron configuration space $(\mathbf{m}_p, \mathbf{m}_n)$, then the first term of the expansion is just the average of this operator in the $(\mathbf{m}_p, \mathbf{m}_n)$ space. This average should involve only the scalars n_r^p, n_r^n ($r = 1, \ldots l$, l is the number of orbits) of the

$$\left[\sum_{j=1}^{l} U_p(N_j) \oplus \sum_{j=1}^{l} U_n(N_j) \right]$$

group. Thus in (10) only the $\nu = 0$ term which give rise to the proton and neutron numbers contributes with

$$[t = r \quad \text{and} \quad u = s \quad \text{and} \quad U(r_j s_j r_j s_j; 10) = \sqrt{3}(-1)^{r_j + s_j - 1}/[r_j]^{\frac{1}{2}}[s_j]^{\frac{1}{2}}]$$

and

$$[n_r = ((a^\dagger)^{rj} \times a^{rj})^0/[r_j]^{\frac{1}{2}} \quad \text{where} \quad [r_j] = (2r_j + 1)]$$

and gets (8) from (10).

For nuclei with $N \neq Z$, the total strength $K(E; mTM_T \to mT'M_T')$ from the initial state with energy E, valence particle number m and isospin T(z-component M_T) to all final states with isospin T' (z-component $M_{T'}$) is given by (Sarkar and Kar 1988a)

$$\begin{aligned} K(E; mTM_T \to mT'M_T') &= [3/(2T'+1)]^{\frac{1}{2}} (C_{M_T M_T' - M_T M_T'}^{T1T'})^2 (-1)^{T'-1-T} \\ &\quad \times \sum_{w_T} (-1)^{w_T} U(T1T1; T' w_T) \Bigg[\langle m, T \| (\bar{O}_{\mathrm{GT}}^{11} \times O_{\mathrm{GT}}^{11})^{0, w_T} \| m, T \rangle \\ &\quad + \left\langle m, T \| (\bar{O}_{\mathrm{GT}}^{11} \times O_{\mathrm{GT}}^{11})^{0, w_T} \frac{(H - E_c(m,T))}{\sigma(m,T)} \| m, T \right\rangle \frac{(E - E_c(m,T))}{\sigma(m,T)} \Bigg], \end{aligned} \tag{11}$$

where $E_c(m, T)$ and $\sigma(m, T)$ are the centroid and the width of the hamiltonian in the (m, T) space. Extension of (11) to configuration spaces is also available.

In table 1 we show the splitting of the β^- strength sums evaluated for some isotopes of Fe and Ni by spectral distribution theory keeping only the first term in (11) and

Table 1. Scalar and configuration averaged β^- strength sum for some Fe and Ni isotopes with decomposition according to the final isospin along with the available shell model values (taken from Bloom and Fuller 1985).

	Spectral distribution method								
	Scalar				Configuration				
Nucleus	$T-1$	T	$T+1$	Total	$T-1$	T	$T+1$	Total	Shell-model total
^{54}Fe	6·77	8·26	1·80	16·83	6·89	8·48	1·88	17·25	15·1
^{56}Fe	14·89	5·53	0·60	21·02	15·44	5·87	0·67	21·98	22.1
^{58}Ni	7·17	8·86	2·00	18·03	7·62	9·49	2·22	19·33	16·6
^{60}Ni	15·25	5·73	0·64	21·62	16·50	6·24	0·77	23·51	24·6
^{60}Fe	26·31	2·98	0·12	29·41	28·09	3·14	0·16	31·39	33·47
^{64}Fe	36·26	1·52	0·02	37·80	37·65	1·48	0·03	39·16	37·16

Table 2. $\eta(E_g)$ of (5) evaluated for ^{20}Ne, ^{24}Mg and ^{28}Si with Gamow-Teller and $M1^{\Delta T=1}$ operators.

Nucleus	$\eta(E_g)$ for	
	GT	Isovector M1
^{20}Ne	0·38	0·06
^{24}Mg	0·53	0·37
^{28}Si	0·61	0·54

compare the total of all three final isospins to the results of a shell model calculation (Bloom and Fuller 1985). The agreement is seen to be reasonably good.

3.2(ii) *GT and $M1^{T=1}$ strength sums in (sd)-shell—case with large positive correlation coefficient*: The correlation coefficient of $O^+_{GT}\ O_{GT}$ with the universal-*sd* interaction for the nuclei ^{20}Ne, ^{24}Mg and ^{28}Si are 0·55, 0·60 and 0·59. For M1 isovector operator, which is very similar to the Gamow-Teller operator except for a small orbital contribution, the correlation coefficient for these three nuclei has values 0·34, 0·48 and 0·53 respectively. The GT strength sums for them with only the first term in the expansion are 5·0, 8·1 and 9·1 respectively whereas retaining terms upto CLT makes them 0·7, $-0·8$ and $-1·4$! For M1 strength sum also we encounter similar problems. But evaluation of η_{K-H-H} and consequently the parameter $\eta(E_g)$ makes it clear that in these cases one needs to take into account the term beyond the CLT limit for both GT and M1. Table 2 gives $\eta(E_g)$ for the Gamow-Teller and $M1^{T=1}$ excitations which are clearly not very small compared to 1. In table 3 we show the total GT and isovector M1 strength sums including the contributions from P_2 $(E_{g.s.})$ (Sarkar and Kar 1988b) and compare them with shell model calculations. The large value of ζ_{K-H} makes clear why the expressions in (8) fail in the (*sd*)-shell. We also mention that earlier efforts (Halemane and French 1982) in evaluating $M1^{T=1}$ strength sums by spectral distributions did not go beyond the CLT and had difficulty as a few numbers came out negative.

Table 3. Gamow-Teller and isovector M1 strength sums for ground states of ^{20}Ne, ^{24}Mg and ^{28}Si evaluated by spectral distribution methods compared to shell model results and estimates for GT using (8) with occupation number expectation values from full shell model (ON), taken from Hino *et al* (1987, 1988).

Nucleus	Strength sum for				
	GT			Isovector M1	
	ON approximation	Spectral distribution	Shell model	Spectral distribution	Shell model
^{20}Ne	4·99	2·35	0·55	5·86	2·57
^{24}Mg	8·22	3·95	2·33	9·92	6·58
^{28}Si	9·71	4·97	3·89	13·29	9·76

Finally we mention some results in the calculation of the strength distribution $R(E, E')$ of (6). The $R(E, E')$ strength in (sd)-shell for ^{21}Mg was worked out retaining terms upto CLT (Kar 1981). In fp-shell, calculations for ^{48}Mn retaining only the first terms in (8) find the centroid of the strength distribution at an excitation energy of 20 MeV for final isospin $T' = 1$ whereas shell model calculations find the peak for $T' = 1$ around 14 MeV. Work to incorporate the effects of the higher term on the expansion is in progress.

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