Chapter 5

Non-Interacting Particle Strength Densities for One-Body Transition Operators

5.1 Introduction

Going beyond state (level) and expectation value densities, the present chapter and the following chapter deal with bivariate strength densities and in particular Gamow - Teller (GT) strength densities are constructed for calculating GT summed strengths and β-decay rates; the bivariate strength density $\mathbf{I}_{\mathcal{O}}^{H}(E,E')$ as stated in Chapter 2, for a transition operator $\mathcal{O}$ and hamiltonian H is the transition strength weighted by the state densities at initial and final energies. The present work is based on the convolution result for strength densities in SAT-LSS. Using some plausible arguments and applying the bivariate Gaussian form (2.15) for $\mathbf{I}_{\mathcal{O}}^{H}$ locally, it was shown by French et al [Fr-87a, Fr-88b] that the IP strength density takes a simple bivariate convolution form, $\mathbf{I}_{\mathcal{O}}^{H}(E,E') = \sum_{S} \mathbf{I}_{\mathcal{O}}^{\mathbf{h},S} \otimes \rho_{\mathcal{O};BIV-\mathcal{G}}^{\mathbf{V},S}[E,E']$. Leaving aside the question of determining the five parameters (two centroids, two variances and the bivariate correlation coefficient) of $\rho^{\mathbf{V}}_{\mathcal{O};BIV-\mathcal{G}}$, one needs good methods for constructing $\mathbf{I}^{\mathbf{h}}_{\mathcal{O}}$ and its S - decompositions in large spaces. This chapter deals with the problem of constructing NIP densities $\mathbf{I}^{\mathbf{h}}_{\mathcal{O}}$ and the next chapter deals with the IP convolution. Therefore without loss of generality, from now on $\mathbf{h}$ is replaced by h. A theory for constructing NIP strength densities, for a general transition operator, is worked out in [Fr-88b] by employing s.p. *states* both for defining the eigen states of h and the transition operator; the NIP strength density takes a bivariate convolution form where one of the factors is a NIP state density and the other a δ function. An alternative formalism is developed in the present chapter using spherical/unitary orbits and spherical tensor form for the transition operators. Here the NIP strength density is written as a superposition of unitary configuration partial densities (they in turn give the S - decompositions required for incorporating interactions) and the partial strength densities are constructed in terms of their low order bivariate moments as Edgeworth corrected Gaussians (2.21) - i.e. CLT is used for the partial strength densities. In statistical spectroscopy studies, bivariate densities are directly constructed in terms of the bivariate moments (i.e. moment method is used) and applied for the first time in [Ko-84a, Ko-85]. The moment method, though approximate (it is exact with spherical configurations) is much faster as the number of unitary orbits is usually much smaller than the corresponding s.p. states. The results of the present chapter are restricted to one-body transition operators. In the next chapter the NIP strength densities for $GT(\beta^-)$ operator are employed in constructing the corresponding IP densities and with this a method for calculating β-decay rates for neutron excess fp-shell nuclei which play an important role in the evolution of massive presupernova stars [Au-90, Au-94], is developed and applied. We will now give a preview.

Sects. 5.2 and 5.3 give preliminaries regarding one-body transition operators $\mathcal{O}^k_\mu$ of spherical tensor rank-k and the NIP strength densities $\mathbf{I}^h_\mathcal{O}$ respectively. In Sect. 5.4 exact expression for $\mathbf{I}^h_\mathcal{O}$ is derived using spherical configurations $\mathbf{m}$. The S decomposition of $\mathbf{I}^h_\mathcal{O}$ and further decomposition into partial unitary configuration densities $\mathbf{I}^{h;[\mathbf{m}],[\mathbf{m}']}_\mathcal{O}$ are introduced in Sect. 5.5. In Sect. 5.6, trace propagation formulas for the bivariate strength density moments M_{rs} for $r+s \leq 4$, for $\mathbf{I}^h_\mathcal{O}$ in m-particle scalar spaces are given; they are used in studying some general features of $\mathbf{I}^h_\mathcal{O}$. In Sect. 5.7, derived are the trace propagation formulas for the various fixed - [m] basic traces that determine the bivariate moments $M_{rs}([\mathbf{m}],[\mathbf{m}'])$ for $r+s \leq 2$, of $\mathbf{I}^{h;[\mathbf{m}],[\mathbf{m}']}_\mathcal{O}$. In Sect. 5.8 a numerical test, in a large shell model space example, for the goodness of bivariate Gaussian representation for the partial NIP strength densities $\mathbf{I}^{h;[\mathbf{m}],[\mathbf{m}']}_\mathcal{O}$ is described. Finally a summary is given in Sect. 5.9. The results given in this chapter are first reported in [Ko-94a].

5.2 One-body transition operators

A general one-body transition operator $\mathcal{O}^k_\mu$ and some of its properties are,

$$
\begin{aligned}
\mathcal{O}^k_\mu &= \sum \epsilon^{(k)}_{\alpha\beta}\left(a^\dagger_\alpha \tilde{a}_\beta\right)^k_\mu = \sum \epsilon^{(k)}_{\alpha\beta}\mathcal{O}^k_{\alpha\beta;\mu}\;, \\
\left(\mathcal{O}^k_\mu\right)^\dagger &= \sum (-1)^{j_\alpha - j_\beta}\epsilon^{(k)}_{\alpha\beta}(-1)^\mu\left(a^\dagger_\beta \tilde{a}_\alpha\right)^k_{-\mu}\;, \\
\left(\mathcal{O}^\dagger\right)^k_\mu &= \sum \epsilon^{(k)}_{\alpha\beta}(-1)^{j_\alpha - j_\beta}\left(a^\dagger_\beta \tilde{a}_\alpha\right)^k_\mu\;, \\
\left(\mathcal{O}^k_\mu\right)^\dagger &= (-1)^\mu\left(\mathcal{O}^\dagger\right)^k_{-\mu}\;,
\end{aligned}
$$

$$\sum_{\mu}\left(\mathcal{O}_{\mu}^{k}\right)^{\dagger}\mathcal{O}_{\mu}^{k} = \left(\mathcal{O}^{\dagger}\right)^{k}\cdot\mathcal{O}^{k}\,. \tag{5.1}$$

In (5.1) $\epsilon_{\alpha\beta}^{(k)}$ are parameters that define $\mathcal{O}_{\mu}^{k}$ and for hermitian $\mathcal{O}$ (i.e. $\left(\mathcal{O}_{\mu}^{k}\right)^{\dagger} = (-1)^{\mu}\mathcal{O}_{-\mu}^{k}$) one has $\epsilon_{\beta\alpha}^{(k)} = (-1)^{j_\alpha - j_\beta}\epsilon_{\alpha\beta}^{(k)}$. For later convenience $\mathcal{O}_{\mu}^{k}$ are divided into four categories and they are

$$\begin{aligned}
[A]:\ \mathcal{O}_{\mu}^{k} &= \sum\epsilon_{\alpha\beta}^{(k)}\left(a_{\alpha_x}^{\dagger}\tilde{a}_{\beta_y}\right)_{\mu}^{k}\ ; \qquad x,y = \text{p or n}\\
[B]:\ \mathcal{O}_{\mu}^{k} &= \alpha_p\left(\mathcal{O}_{\mu}^{k}\right)_p + \alpha_n\left(\mathcal{O}_{\mu}^{k}\right)_n\\
[C]:\ \mathcal{O}_{\mu}^{k} &= \sum\epsilon_{\alpha_p\beta_n}^{(k)}\left(a_{\alpha_p}^{\dagger}\tilde{a}_{\beta_n}\right)_{\mu}^{k}\\
[D]:\ \mathcal{O}_{\mu}^{k} &= \sum\epsilon_{\alpha_n\beta_p}^{(k)}\left(a_{\alpha_n}^{\dagger}\tilde{a}_{\beta_p}\right)_{\mu}^{k}
\end{aligned} \tag{5.2}$$

In (5.2), α_p and α_n are parameters. The operator $\mathcal{O}_{\mu}^{k}$ under category [A] belongs to identical particle system (protons or neutrons) while the remaining three are for pn systems. Note that electromagnetic operators belong to category [B] while $GT(\beta^+)$ and $GT(\beta^-)$ operators belong to categories [C] and [D] respectively. For example, explicit expressions for $GT(\beta^{\pm})$ operator and the corresponding $\epsilon_{\alpha\beta}^{(k)}$'s are,

$$\mathcal{O}_{GT(\beta^{\pm})} = \sum\epsilon_{\alpha(n'\ell'\frac{1}{2}j'),\beta(n\ell\frac{1}{2}j)}^{(1)}\left(a_{\alpha_x}^{\dagger}a_{\beta_y}\right)_{\mu}^{1}\ ;$$

$$x = \text{n},\quad y = \text{p}\ \text{ for }\ \beta^{+}\ \text{and}\ x = \text{p},\quad y = \text{n}\ \text{ for }\ \beta^{-}\,,$$

$$\epsilon_{\alpha\beta}^{(1)} = \epsilon_{\alpha(n'\ell'\frac{1}{2}j'),\beta(n\ell\frac{1}{2}j)}^{(1)}$$

$$= \delta_{\ell\ell'}\delta_{nn'}\sqrt{\frac{2j+1}{3}}\frac{[j(j+1)+3/4-\ell(\ell+1)]}{\sqrt{j(j+1)}}\ ;\ \text{ for }\ j = j'$$

$$\epsilon_{\alpha\beta}^{(1)} = \epsilon_{\alpha(n'\ell'\frac{1}{2}j'),\beta(n\ell\frac{1}{2}j)}^{(1)} = \delta_{\ell\ell'}\delta_{nn'}(\pm)\sqrt{\frac{8\ell(\ell+1)}{3(2\ell+1)}}\ ;\,.$$

$$\pm\ \text{ for }\ j = \ell\pm\frac{1}{2}\ \text{ and }\ j' = \ell\mp\frac{1}{2} \tag{5.3}$$

In (5.3), (n, n') denote the oscillator radial quantum numbers, i.e. for oscillator shell N, $2n+\ell = N$. The delta functions in (5.3) for $\epsilon^{(1)}_{\alpha\beta}$ show that the $\mathcal{O}_{GT(\beta\pm)}$ operator is S-conserving when S quantum number is defined by the oscillator $n\hbar\omega$ excitations. Appendix D gives the explicit expressions for electromagnetic multiple operators and the corresponding $\epsilon^{(k)}_{\alpha\beta}$'s.

5.3 NIP strength densities

Given a NIP hamiltonian $h = \sum \epsilon_\alpha n_\alpha$ and a transition operator $\mathcal{O}^k_\mu$, explicit definitions of the strength $R^h_{\mathcal{O}}(E, E')$ and the strength density $\mathbf{I}^h_{\mathcal{O}}(E, E')$ follow from (2.36) and (2.37); in these equations, a factor $(2k+1)$ is used for convenience. In the NIP case the eigenstates are labelled by spherical configurations $\mathbf{m}$ with energies $\epsilon(\mathbf{m}) = \sum \epsilon_\alpha m_\alpha$ and degeneracies $d(\mathbf{m}) = \prod_\alpha \begin{pmatrix} N_\alpha \\ m_\alpha \end{pmatrix}$. Then $\mathbf{I}^h_{\mathcal{O}}(E, E')$ is given by

$$\mathbf{I}^h_{\mathcal{O}}(E, E') = (2k+1)^{-1} \sum_{\mathbf{m},\mathbf{m}',\mu} \sum_{\substack{\gamma \in \mathbf{m} \\ \gamma' \in \mathbf{m}'}} \left| \langle \mathbf{m}'\gamma' | \mathcal{O}^k_\mu | \mathbf{m}\gamma \rangle \right|^2 \delta(E - \epsilon(\mathbf{m}))\delta(E' - \epsilon(\mathbf{m}')) \tag{5.4}$$

In order to construct the total NIP density $\mathbf{I}^h_{\mathcal{O}}(E, E')$ and carry out its S - decompositions, strength densities are generated using : (i) spherical configurations, p or n or (p and n); (ii) scalar m - particle space, p or n; (iii) unitary configurations, p or n or (p and n). These three cases are dealt with in Sects. 5.4, 5.6 and 5.7 respectively.

5.4 Exact expression for $\mathbf{I}_{\mathcal{O}}^{h}$: spherical configurations

5.4.1 Identical particles

In order to derive the exact formula for $\mathbf{I}_{\mathcal{O}}^{h}$, first one should recognize that in (5.4) the summation over (m, m′) configurations disappears (i.e. when one is using spherical configuration decomposition of the m - particle spaces) as they are uniquely defined by E and E' respectively; from now on in this section, the summation over (m, m′) is dropped. As the transition operators that are being considered are of one-body $(a_\alpha^\dagger a_\beta)$ type, in general there are two types of strengths possible which are denoted by $\Delta = 0$ (m = m′) and 1 (m ≠ m′) respectively. In both cases as we shall see ahead, the strength density is reduced to a trace over the initial configuration (m). First the case of identical particles is considered; here one is using only category [A] operators of (5.2).

In $\Delta = 0$ case m′ = m, i.e. the initial and final configurations are same. Then only the part $\left[\sum_{\mu} \epsilon_{\alpha\alpha}^{(k)} \mathcal{O}_{\alpha\alpha;\mu}^{k}\right]$ of $\mathcal{O}_{\mu}^{k}$ will contribute to the strength,

$$\begin{aligned}\mathbf{I}_{\mathcal{O}}^{h}(E,E') &= (2k+1)^{-1} d(\mathrm{m}) \left\langle \left(\sum_{\alpha} \epsilon_{\alpha\alpha}^{(k)} \mathcal{O}_{\alpha\alpha}^{\dagger}\right)^{k} \cdot \left(\sum_{\alpha'} \epsilon_{\alpha'\alpha'}^{(k)} \mathcal{O}_{\alpha'\alpha'}^{k}\right)\right\rangle^{\mathrm{m}} \\ &\quad \times \delta(E-\epsilon(\mathrm{m}))\delta(E'-\epsilon(\mathrm{m}))\end{aligned} \tag{5.5}$$

The trace in (5.5) is evaluated by decomposing $\left(\sum_{\alpha} \epsilon_{\alpha\alpha}^{k} \mathcal{O}_{\alpha\alpha}^{\dagger}\right)^{k} \cdot \left(\sum_{\alpha'} \epsilon_{\alpha'\alpha'}^{k} \mathcal{O}_{\alpha'\alpha'}^{k}\right)$ into one and two-body parts and only the TBME of the type $V_{\alpha\beta\alpha\beta}^{k'}$ will contribute to the configuration trace. The resulting SPE ϵ_α' and TBME $V_{\alpha\beta\alpha\beta}^{k'}$ are $\epsilon_\alpha' = \sum_{\alpha} \left[\left\{\epsilon_{\alpha\alpha}^{(k)}\right\}^2 / N_\alpha\right] n_\alpha$ and $V_{\alpha\beta\alpha\beta}^{k'} = 2(-1)^{j_\alpha + j_\beta - k'} \epsilon_{\alpha\alpha}^{(k)} \epsilon_{\beta\beta}^{(k)} \left\{\begin{matrix} j_\alpha & j_\alpha & k \\ j_\beta & j_\beta & k' \end{matrix}\right\}$.

Using these and evaluating the fixed-m trace in (5.5), gives

$$\mathbf{I}^h_{\mathcal{O}}(E,E') = d(\mathbf{m})\delta(E-\epsilon(\mathbf{m}))\delta(E'-\epsilon(\mathbf{m}))\times$$

$$\left\{\left[\sum_{\alpha}\frac{\left\{\epsilon^{(k)}_{\alpha\alpha}\right\}^2}{N_\alpha}m_\alpha(\mathbf{m})\right]+\left[\sum_{\alpha>\beta}2(\epsilon^{(k)}_{\alpha\alpha}\epsilon^{(k)}_{\beta\beta})\delta_{k,0}\times m_\alpha(\mathbf{m})m_\beta(\mathbf{m})\right]+\right.$$

$$\left.\left[\sum_{\alpha}2\frac{\left\{\epsilon^{(k)}_{\alpha\alpha}\right\}^2}{N_{\alpha\alpha}}\left[\sum_{k'=0,2,4,..}(-1)^{1+k'}(2k'+1)\left\{\begin{array}{ccc} j_\alpha & j_\alpha & k \\ j_\alpha & j_\alpha & k'\end{array}\right\}\right]m_{\alpha\alpha}(\mathbf{m})\right]\right\}$$

(5.6)

Simplifying the summation involving the six-j symbol in (5.6) leads to, for $k \neq 0$, the following compact expression for $\mathbf{I}^h_{\mathcal{O}}(E,E')$,

$$\mathbf{I}^h_{\mathcal{O}}(E,E') = d(\mathbf{m})\sum_{\alpha}\left\{\epsilon^{(k)}_{\alpha\alpha}\right\}^2\{m_\alpha(\mathbf{m})m^\times_\alpha(\mathbf{m})N^{-1}_{\alpha\alpha}\}\delta(E-\epsilon(\mathbf{m}))\delta(E-E') \tag{5.7}$$

In (5.7), $m_\alpha(\mathbf{m})$ gives number of particles in orbit α for the configuration $\mathbf{m}$ and similarly $m^\times_\alpha(\mathbf{m})$ is defined.

In $\Delta = 1$ case only the terms $a^\dagger_\alpha a_\beta$ with $\alpha \neq \beta$ will contribute i.e. in the configuration $\mathbf{m}$, a particle in orbit β is destroyed and a particle in orbit α (with $\alpha \neq \beta$) is created, leading to $\mathbf{m}'$. Then $\mathbf{m}'$ is uniquely defined by $\mathbf{m}$ and (α,β); $\mathbf{m}' = \mathbf{m}\times\left(1^\dagger_\alpha 1_\beta\right)$. Alternatively given the initial configuration $\mathbf{m}$ and final configuration $\mathbf{m}'$, a unique $\mathcal{O}^k_{\alpha\beta}$ term will contribute to the strength. With this, $\mathbf{I}^h_{\mathcal{O}}(E,E')$ is given by

$$\mathbf{I}^h_{\mathcal{O}}(E,E') = (2k+1)^{-1}d(\mathbf{m})\left\{\epsilon^{(k)}_{\alpha\beta}\right\}^2\left\langle\left(\mathcal{O}^\dagger_{\alpha\beta}\right)^{(k)}\cdot\mathcal{O}^k_{\alpha\beta}\right\rangle^{\mathbf{m}}\times$$

$$\delta(E-\epsilon(\mathbf{m})\delta(E'-\epsilon[(\mathbf{m}')=(\mathbf{m})\times(1^\dagger_\alpha 1_\beta)]) \tag{5.8}$$

The configuration scalar part of $\left(\mathcal{O}^\dagger_{\alpha\beta}\right)^k\cdot\mathcal{O}^k_{\alpha\beta}$ is $(2k+1)n_\beta n^\times_\alpha/N_{\beta\alpha}$ and with this the formula for $\mathbf{I}^h_{\mathcal{O}}$ in (5.8) is,

$$\mathbf{I}^h_{\mathcal{O}}(E,E') = d(\mathbf{m})\left\{\epsilon^{(k)}_{\alpha\beta}\right\}^2\{m_\beta(\mathbf{m})\}\{m^\times_\alpha(\mathbf{m})\}\left[N_{\beta\alpha}\right]^{-1}\times$$

$$\delta(E-\epsilon(\mathrm{m}))\delta\left(E'-\epsilon\left[(\mathrm{m}')=(\mathrm{m})\times\left(1^\dagger_\alpha 1_\beta\right)\right]\right) . \tag{5.9}$$

Combining (5.7, 5.9), the general expression for the exact NIP density $\mathbf{I}^h_{\mathcal{O}}$ is,

$$\begin{aligned}\mathbf{I}^h_{\mathcal{O}}(E,E') &= d(\mathrm{m})\sum_{\alpha,\beta}\left\{\epsilon^{(k)}_{\alpha\beta}\right\}^2\{m_\beta(\mathrm{m})\}\{m^\times_\alpha(\mathrm{m})\}N^{-1}_{\beta\alpha}\times \\ &\quad \delta(E-\epsilon(\mathrm{m}))\delta(E'-\epsilon\left[(\mathrm{m}')=(\mathrm{m})\times\left(1^\dagger_\alpha 1_\beta\right)\right]) .\end{aligned} \tag{5.10}$$

5.4.2 pn systems

For pn systems, and for transition operators that belong to category [B] of (5.2), $\mathcal{O}^k_\mu = e_p(\mathcal{O}^k_\mu)_p + e_n(\mathcal{O}^k_\mu)_n$ and the strength density involve $(\mathcal{O}^k_\mu)^\dagger(\mathcal{O}^k_\mu) = e^2_p(\mathcal{O}^k_\mu)^\dagger_p(\mathcal{O}^k_\mu)_p + e^2_n(\mathcal{O}^k_\mu)^\dagger_n(\mathcal{O}^k_\mu)_n + e_pe_n(\mathcal{O}^k_\mu)^\dagger_p(\mathcal{O}^k_\mu)_n + e_ne_p(\mathcal{O}^k_\mu)^\dagger_n(\mathcal{O}^k_\mu)_p$ with a trace over $(\mathrm{m}_p, \mathrm{m}_n)$. Obviously for $k \neq 0$, the pn cross terms will vanish as they cannot be reduced to a configuration scalar. Then, with only the pp and nn terms surviving, the expression for $\mathbf{I}^h_{\mathcal{O}}$ is given by (5.10) with the conventions defined in Sect. 3.1.5 for the orbit (α) indices. For pn one-body transition operators that belong to categories [C] and [D] (5.2), only the $\Delta = 1$ case discussed in Sect. 5.4.1 will be relevant as here $\alpha \neq \beta$ (one of them being a proton index and other a neutron index). Therefore just as above, in this case also (5.10) will give the exact NIP strength density with the conventions for the orbit indices (α) given in Sect. 3.1.5.

Thus for all the four categories of one-body operators given in (5.2), the exact $\mathbf{I}^h_{\mathcal{O}}$ *can be constructed using (5.10) and the conventions given in Sect. 3.1.5 for orbit indices.*

5.5 S-decomposition of strength densities

The strength density $\mathbf{I}^h_{\mathcal{O}}(E,E')$ can be decomposed into unitary orbit densities and also into fixed-S densities which will then allow us to apply the IP formalism for strength densities ([Fr-87a, Fr-88b, Ko-94b]) in very large spaces. To this end (5.4) is rewritten as,

$$\begin{aligned}
\mathbf{I}^{h;m}_{\mathcal{O}}(E,E') &= \sum_{[\mathrm{m}],[\mathrm{m}']}\left[\sum_{\mathrm{m}\in[\mathrm{m}],\,\mathrm{m}'\in[\mathrm{m}']} \overline{|\langle \mathrm{m}'|\mathcal{O}^k|\mathrm{m}\rangle|^2} I^{h,\mathrm{m}}(E) I^{h,\mathrm{m}'}(E')\right] \\
&= \sum_{[\mathrm{m}],[\mathrm{m}']} [\mathbf{I}^{h;[\mathrm{m}],[\mathrm{m}']}_{\mathcal{O}}(E,E')] \\
&= \sum_{S,S'} \mathbf{I}^{h;\,S,S'}_{\mathcal{O}}(E,E')\ ; \\
\mathbf{I}^{h;\,S,S'}_{\mathcal{O}}(E,E') &= \sum_{\substack{[\mathrm{m}]\in S\\ [\mathrm{m}']\in S'}} \mathbf{I}^{h;\,[\mathrm{m}],[\mathrm{m}']}_{\mathcal{O}}(E,E')\ ; \\
I^{h;\,\mathrm{m}}(E) &= d(\mathrm{m})\delta(E-\epsilon(\mathrm{m})) \\
\overline{|\langle \mathrm{m}'|\mathcal{O}^k|\mathrm{m}\rangle|^2} &= (2k+1)^{-1}\sum_{\gamma,\gamma',\mu} \frac{|\langle \mathrm{m}'\gamma'|\mathcal{O}^k_\mu|\mathrm{m}\gamma\rangle|^2}{d(\mathrm{m})d(\mathrm{m}')}
\end{aligned} \tag{5.11}$$

Eq. (5.11) applies directly to pn case. The first two equalities in (5.11) define the unitary configuration partial strength densities $\mathbf{I}^{h;[\mathrm{m}],[\mathrm{m}']}_{\mathcal{O}}$ and the next two equalities define the S - decomposition, i.e. $\mathbf{I}^{h;S,S'}_{\mathcal{O}}$. The bivariate moments $\mathbf{M}_{PQ}$ of the unitary orbit strength densities $\mathbf{I}^{[\mathrm{m}],[\mathrm{m}']}_{\mathcal{O}}(E,E')$ are,

$$\begin{aligned}
\mathbf{M}_{PQ}([\mathrm{m}],[\mathrm{m}']) &= [d([\mathrm{m}])]^{-1}\times \\
&\qquad \sum_{\substack{\mathrm{m}\in[\mathrm{m}]\\ \mathrm{m}'\in[\mathrm{m}']}} \overline{|\langle \mathrm{m}'|\mathcal{O}^k|\mathrm{m}\rangle|^2}\times[d(\mathrm{m})d(\mathrm{m}')\epsilon^P(\mathrm{m})\epsilon^Q(\mathrm{m}')] \\
&= (2k+1)^{-1}\sum_\mu \langle (\mathcal{O}^k_\mu)^\dagger \mathbf{P}([\mathrm{m}'])h^Q\mathcal{O}^k_\mu h^P\rangle^{[\mathrm{m}]}
\end{aligned}$$

$$= [(2k+1)d([\mathrm{m}])]^{-1} \sum_{\mu,\gamma,\gamma'} \langle [\mathrm{m}]\gamma | \left(\mathcal{O}^k_\mu\right)^\dagger |[\mathrm{m}']\gamma'\rangle\langle[\mathrm{m}']\gamma'|h^Q\mathcal{O}^k_\mu h^P|[\mathrm{m}]\gamma\rangle \; ;$$

$$\mathbf{P}([\mathrm{m}'])|[\mathrm{m}]\gamma\rangle = |[\mathrm{m}']\gamma\rangle\delta_{[\mathrm{m}],[\mathrm{m}']} \qquad (5.12)$$

In (5.12), $\mathbf{P}([\mathrm{m}'])$ is a projection operator. The first equality in (5.12) together with (5.10) (i.e. using the exact NIP density) one can numerically calculate the bivariate moments $\mathbf{M}_{PQ}$. However using the second and third equalities in (5.12), it is possible to derive propagation equations for the $\mathbf{M}_{PQ}$ traces directly in terms of (without using spherical configurations) the unitary configuration labels. We will do this in the next two sections. It must be mentioned that the $\mathbf{M}_{PQ}$ defined in (5.12) are not normalized and in order to construct an Edgeworth (bivariate) representation of $\mathbf{I}_{\mathcal{O}}^{[\mathrm{m}],[\mathrm{m}']}(E,E')$ one should use the normalized moments M_{PQ},

$$M_{PQ}([\mathrm{m}],[\mathrm{m}']) \;=\; \mathbf{M}_{PQ}([\mathrm{m}],[\mathrm{m}'])/\mathbf{M}_{00}([\mathrm{m}],[\mathrm{m}']) \qquad (5.13)$$

$$\mathbf{I}_{\mathcal{O}}^{[\mathrm{m}],[\mathrm{m}']}(E,E') \;=\; \mathbf{M}_{00}([\mathrm{m}],[\mathrm{m}'])\rho_{\mathcal{O}}^{[\mathrm{m}],[\mathrm{m}']}(E,E'), \qquad (5.14)$$

where ρ is normalized bivariate density. Explicit expression for bivariate Edgeworth corrected Gaussian is given in (2.21).

As an example using $GT(\beta^-)$ operator and choosing the s.p. orbits $[1d_{5/2}, 2s_{1/2}, 1d_{3/2}]$ and $[1f_{7/2}, 2p_{3/2}, 1f_{5/2}, 2p_{1/2}]$ to be the unitary orbits (denoted by # 1, 2) for both protons and neutrons and SPE (in MeV) to be Seeger [Hi-69] energies 16.388, 20.596, 21.851, 24.752, 29.431, 31.208, 32.201 respectively for the seven spherical orbits, the bivariate reduced cumulants k_{rs} are calculated for the strength densities $\mathbf{I}_{\mathcal{O}(GT)}^{h;[\mathrm{m}],[\mathrm{m}']}$ with $(m_p,m_n)=(4,6) \rightarrow (m_p',m_n')=(5,5)$ and $S=S'=0$, 1 and 2. Here Eqs. (5.3, 5.10, 5.12, 5.13, 2.18) are used. It is seen that the bivariate cumulants k_{rs} for $r+s \geq 3$ are usually small. With $\{m_1,m_2,m_3,m_4\}$ denoting a unitary configuration with m_1 protons in $\#1, m_2$

protons in #2, m_3 neutrons in #1 and m_4 neutrons in #2 ($m_p = m_1 + m_2$, $m_n = m_3 + m_4$), the cumulants k_{rs} for $r + s \geq 3$ are: for $[4,0,6,0] \rightarrow [5,0,5,0]$ with $S = 0 \rightarrow S' = 0$, $k_{03} = 0.008$, $k_{04} = -0.11$, $k_{12} = 0.006$, $k_{13} = -0.07$, $k_{21} = 0.005$, $k_{22} = -0.09$, $k_{30} = -0.007$, $k_{31} = -0.08$ and $k_{40} = -0.11$; for $[4,0,5,1] \rightarrow [4,1,5,0]$ with $S = 1 \rightarrow S' = 1$, $k_{03} = -0.01$, $k_{04} = -0.14$, $k_{12} = 0.0004$, $k_{13} = -0.07$, $k_{21} = 0.0004$, $k_{22} = -0.07$, $k_{30} = -0.01$, $k_{31} = -0.07$ and $k_{40} = -0.14$; for $[3,1,5,1] \rightarrow [4,1,4,1]$ with $S = 2 \rightarrow S' = 2$, $k_{03} = -0.02$, $k_{04} = -0.16$, $k_{12} = -0.02$, $k_{13} = -0.14$, $k_{21} = -0.02$, $k_{22} = -0.15$, $k_{30} = -0.02$, $k_{31} = -0.14$ and $k_{40} = -0.16$. In this example the widths are $\simeq 6 - 7$ MeV and the correlation coefficients $\zeta = k_{11} \simeq 0.8$.

5.6 Scalar strength density bivariate moments: identical particles

In the scalar (m - particle average case) only the identical particle case is relevant with category [A] operators given in (5.2). As here $[\mathrm{m}] = m = [\mathrm{m}']$, the bivarite moments $\mathbf{M}_{PQ}([\mathrm{m}],[\mathrm{m}'])$ are written as $\mathbf{M}_{PQ}(m)$. The moments $\mathbf{M}_{PQ}(m)$ are expressible in terms of $\widetilde{M}_{PQ}(m)$ which are defined by $\widetilde{M}_{PQ}(m) = (2k+1)^{-1} \sum_{\mu} \langle (O^k_\mu)^\dagger \tilde{h}^Q O^k_\mu) \tilde{h}^P \rangle^m$; $h = \sum \epsilon_\alpha n_\alpha \Longrightarrow \tilde{h} = \sum \tilde{\epsilon}_\alpha n_\alpha$ and $\tilde{\epsilon}_\alpha = \epsilon_\alpha - \bar{\epsilon}$, $\bar{\epsilon} = (\sum N_\alpha \epsilon_\alpha)/N$ as given in (2.49). Propagation formulas for $\widetilde{M}_{PQ}$ are derived, though tedious but straight forward, using the methods given in detail in Sects. 2.5 - 2.6. With $\mathbf{X}_{PQ}(i)$ denoting the i-body part of $(2k+1)^{-1} \sum_{\mu} (O^k_\mu)^\dagger \tilde{h}^Q O^k_\mu \tilde{h}^P$ and $Z_{PQ}(i) = \langle \mathbf{X}_{PQ}(i) \rangle^i$, the trace propagation formulas for $\widetilde{M}_{PQ}$ for $P+Q \leq 2$ are,

$$\widetilde{M}_{00}(m) = M_{00} = \frac{m m^\times}{[N]_2} Z_{00}(1) \; ; \; Z_{00}(1) = \sum_{\alpha,\beta} \left\{ \epsilon^{(k)}_{\alpha\beta} \right\}^2 \qquad (5.15)$$

$$\widetilde{M}_{10}(m) = \widetilde{M}_{01}(m) = \frac{mm^{\times}(m^{\times}-m)}{[N]_3} Z_{PQ}(1) \; ;$$

$$Z_{10}(1) = Z_{01}(1) = \sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_{\alpha} \tag{5.16}$$

$$\widetilde{M}_{PQ}(m) = \left[\frac{mm^{\times}}{[N]_2} + \frac{[m]_2[m^{\times}]_2}{[N]_4}\right] Z_{PQ}(1) + \left[\frac{[m]_2[m^{\times}]_2}{[N]_4}\right] Z_{PQ}(2) \; ; \; P+Q=2,$$

$$Z_{20}(1) = Z_{02}(1) = \sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_{\alpha}^2$$

$$\begin{aligned} Z_{20}(2) = Z_{02}(2) \;&=\; -5\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_{\alpha}^2 - 2\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_{\alpha}\widetilde{\epsilon}_{\beta} \\ &+\; \left[\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2\right] \left[\sum_{\tau} \widetilde{\epsilon}_{\tau}^2 N_{\tau}\right] \end{aligned}$$

$$Z_{11}(1) = \sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_{\alpha}\widetilde{\epsilon}_{\beta}$$

$$Z_{11}(2) = -4\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_{\alpha}^2 - 3\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_{\alpha}\widetilde{\epsilon}_{\beta} + \left[\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2\right] \left[\sum_{\tau} \widetilde{\epsilon}_{\tau}^2 N_{\tau}\right] \tag{5.17}$$

For $P+Q=3,4$ the basic inputs $Z_{PQ}(i)$ are given in Tables 5.1, 5.2 and they together with the following propagation formulas will determine $\widetilde{M}_{PQ}(m)$ for $P+Q=3,4$,

$$\begin{aligned} \widetilde{M}_{PQ}(m) \;&=\; \left\{\frac{3[m]_2[m^{\times}]_2(m^{\times}-m)}{[N]_5} + \frac{mm^{\times}(m^{\times}-m)}{[N]_3}\right\} Z_{PQ}(1) \\ &+ \left\{\frac{[m]_2[m^{\times}]_2(m^{\times}-m)}{[N]_5}\right\} Z_{PQ}(2) \; ; \quad P+Q=3 \end{aligned} \tag{5.18}$$

$$\begin{aligned} &\widetilde{M}_{PQ}(m) = \left\{\frac{mm^{\times}}{[N]_2} + \frac{[m]_2[m^{\times}]_2}{[N]_4} + \frac{2[m]_3[m^{\times}]_3}{[N]_6}\right\} Z_{PQ}(1) \\ &+ \left\{\frac{[m]_2[m^{\times}]_2}{[N]_4} + \frac{2[m]_3[m^{\times}]_3}{[N]_6}\right\} Z_{PQ}(2) + \left\{\frac{[m]_3[m^{\times}]_3}{[N]_6}\right\} Z_{PQ}(3) \; ; \quad P+Q=4 \end{aligned} \tag{5.19}$$

Table 5.1 Basic inputs $Z_{PQ}(i) = \sum_{r=1}^{4} a_r A_r$ for $\widetilde{M}_{PQ}(m)$ moments with $P+Q = 3$. The a_r's and A_r's are given in the table.

(P,Q)	i	a_r			
		$r=1$	$r=2$	$r=3$	$r=4$
(3,0)	1	1	0	0	0
(3,0)	2	-9	-6	3	1
(2,1)	1	0	1	0	0
(2,1)	2	-6	-9	3	1

$$A_1 = \sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \tilde{\epsilon}_\alpha^3 \qquad A_2 = \sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \tilde{\epsilon}_\alpha^2 \tilde{\epsilon}_\beta$$

$$A_3 = \left[\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \tilde{\epsilon}_\alpha\right]\left[\sum_\tau \tilde{\epsilon}_\tau^2 N_\tau\right] \qquad A_4 = \left[\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2\right]\left[\sum_\tau \tilde{\epsilon}_\tau^3 N_\tau\right]$$

Given the expression for $\widetilde{M}_{PQ}(m)$, the $\mathbf{M}_{PQ}(m)$ moments are easy to write down,

$$\mathbf{M}_{PQ}(m) = \sum_{r=0-P,s=0-Q} \binom{P}{r}\binom{Q}{s} \widetilde{M}_{rs}(m)(m\bar{\epsilon})^{P+Q-r-s} \qquad (5.20)$$

Using the relationship between the normalized moments $M_{PQ} = \mathbf{M}_{PQ}/\mathbf{M}_{00}$, the central moments $\mathcal{M}_{PQ}$ and the cumulants k_{PQ} together with (5.15 - 5.20) one is in a position to construct a bivariate Edgeworth representation (2.21) for $\mathbf{I}_{O}^{h,m}$. Before going to the next section, it should be mentioned that the formulas in (5.15 - 5.20) are verified numerically by using the first equality in (5.12) and (5.10). The scalar propagation equations and the moments $\mathbf{M}_{PQ}(m)$ for

Table 5.2 Basic inputs $Z_{PQ}(i) = \sum_{r=1}^{8} a_r A_r$ for $\widetilde{M}_{PQ}(m)$ moments with $P+Q = 4$. The a_r's and A_r's are given in the table.

(P,Q)	i	a_r							
		$r=1$	$r=2$	$r=3$	$r=4$	$r=5$	$r=6$	$r=7$	$r=8$
(4,0)	1	1	0	0	0	0	0	0	0
(4,0)	2	−17	−8	−6	6	0	4	1	0
(4,0)	3	80	64	36	−36	−12	−24	−8	3
(3,1)	1	0	1	0	0	0	0	0	0
(3,1)	2	−10	−15	−6	3	3	4	1	0
(3,1)	3	68	76	36	−30	−18	−24	−8	3
(2,2)	1	0	0	1	0	0	0	0	0
(2,2)	2	−8	−16	−7	2	4	4	1	0
(2,2)	3	64	80	36	−28	−20	−24	−8	3

$$A_1 = \sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_\alpha^4 \qquad A_2 = \sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_\alpha^3 \widetilde{\epsilon}_\beta$$

$$A_3 = \sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_\alpha^2 \widetilde{\epsilon}_\beta^2 \qquad A_4 = \left[\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_\alpha^2\right] \left[\sum_{\tau} \widetilde{\epsilon}_\tau^2 N_\tau\right]$$

$$A_5 = \left[\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_\alpha \widetilde{\epsilon}_\beta\right] \left[\sum_{\tau} \widetilde{\epsilon}_\tau^2 N_\tau\right] \qquad A_6 = \left[\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2 \widetilde{\epsilon}_\alpha\right] \left[\sum_{\tau} \widetilde{\epsilon}_\tau^3 N_\tau\right]$$

$$A_7 = \left[\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2\right] \left[\sum_{\tau} \widetilde{\epsilon}_\tau^4 N_\tau\right] \qquad A_8 = \left[\sum_{\alpha,\beta} \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2\right] \left[\sum_{\tau_1} \widetilde{\epsilon}_{\tau_1}^2 N_{\tau_1} \sum_{\tau_2} \widetilde{\epsilon}_{\tau_2}^2 N_{\tau_2}\right]$$

$P + Q \leq 4$ are useful for many purposes. For example the expressions (and the methods) for the scalar moments indicate the methods for deriving unitary configuration traces as given ahead in Sect. 5.7. Eqs. (5.15 - 5.20) allow us to study the asymptotic behavior of bivariate correlation coefficients and the higher order shape parameters defined by the bivariate cumulants k_{rs}. As an example let us consider the case of a random one-body hamiltonian $h = \sum \epsilon_\alpha n_\alpha$ with $N_\alpha = 1$ for any α and ϵ_α to be zero centered independent Gaussian random variables with unit variance. With $Y = \sum \left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2$, assuming $\epsilon_{\alpha\alpha}^{(k)} = 0$ and using (5.15, 5.17), give $Z_{00}(1) = Y$, $Z_{20}(1) = Y$, $Z_{20}(2) = Y(N-5)$, $Z_{11}(1) = 0$ and $Z_{11}(2) = Y(N-4)$. In the dilute limit ($m \to \infty$, $N \to \infty$, $m/N \to 0$), they lead to the results that $\zeta(m) \simeq 1 - 1/m$. Therefore in general the NIP state density correlation coefficient will be large – with half a dozen to dozen particles $\zeta \simeq 0.8 - 0.9$ (see also the numerical example in Sect. 5.5). It should be added that it is easy to derive finite - N corrections to the $\zeta(m)$ expression given above. Using (5.15 - 5.20), numerical calculations of the shape parameters k_{rs} (for $r + s = 3, 4$) is straightforward and with k_{rs}, one can have estimates (in finite - (N, m) cases) for departures from the bivariate Gaussian nature; for example, as can be seen from Table 5.3, in the above model, with $N = 40$ and $m = 10$, $k_{11} = 0.87$, $k_{40} = -0.15$, $k_{31} = -0.13$, $k_{22} = 0.12$ and similarly with $N = 100$, $m = 20$ give $k_{11} = 0.94$, $k_{40} = -0.06$, $k_{31} = -0.06$, $k_{22} = 0.05$. A different model where $\epsilon_{\alpha\beta}^{(k)}$ are chosen to be Gaussian random variables was dealt with in [Fr-88b] and this model also gives $\zeta(m) \simeq 1 - 1/m$; Eqs. (5.15 - 5.20) reproduce the results of [Fr-88b] and in addition they give finite - N corrections for the bivariate cumulants.

Table 5.3 Bivariate cumulants (k_{rs}) in scalar space for a random one-body hamiltonian: In the table N is number of single particle states and m is number of particles. Note that in the model considered in the text, $k_{rs} = 0$ for $r + s$ odd.

	$N = 20$		
	$m = 4$	$m = 8$	$m = 10$
$k_{11} = \zeta$	0.70	0.80	0.80
k_{40}	−0.28	−0.31	−0.31
k_{31}	−0.20	−0.25	−0.26
k_{22}	−0.17	−0.23	−0.24
	$N = 40$		
	$m = 4$	$m = 10$	$m = 20$
$k_{11} = \zeta$	0.73	0.87	0.90
k_{40}	−0.13	−0.15	−0.15
k_{31}	−0.09	−0.13	−0.14
k_{22}	−0.08	−0.12	−0.13
	$N = 100$		
	$m = 10$	$m = 20$	$m = 50$
$k_{11} = \zeta$	0.89	0.94	0.96
k_{40}	−0.06	−0.06	−0.06
k_{31}	−0.05	−0.06	−0.06
k_{22}	−0.05	−0.05	−0.06

5.7 Unitary configuration strength density bivariate moments

5.7.1 Identical particles

In the unitary configuration case, propagation equations for the bivariate strength density moments $\widehat{M}_{PQ}([\mathrm{m}])$,

$$\widehat{M}_{PQ}([\mathrm{m}]) = (2k+1)^{-1} \langle \sum_{\mu} (\mathcal{O}^k_\mu)^\dagger h^Q \mathcal{O}^k_\mu h^P \rangle^{[\mathrm{m}]}, \qquad (5.21)$$

with $P+Q \leq 2$ are derived and the results are given below. Their decomposition into partial strength moments $M_{PQ}([\mathrm{m}],[\mathrm{m}'])$ (5.12, 5.13) that define the partial strength densities $\mathbf{I}_{\mathcal{O}}^{h;[\mathrm{m}],[\mathrm{m}']}$ is straight forward and this is described in Sect. 5.7.3. All the discussion below is appropriate for identical particle systems and Sect. 5.7.2 deals with pn systems.

In order to derive propagation formulas for $\widehat{M}_{PQ}([\mathrm{m}])$ traces, the method employed is to first carry out the unitary decomposition (using the results of Sect. 2.5) of the operators $[\ (2K+1)^{-1} \sum\limits_{\mu} (\mathcal{O}_\mu^k)^\dagger \mathcal{O}_\mu^k\ ]$ which is denoted as $\mathcal{O}^\dagger\mathcal{O}$, and h^2. They will have $[\mathbf{0}] \oplus [\mathbf{1}] \oplus [\mathbf{2}]$ unitary tensor parts; only the diagonal TBME of $\mathcal{O}^\dagger\mathcal{O}$ contribute to the $\widehat{M}_{PQ}$ moments. The SPE and TBME of h^2 operator are (note that $h = h^{[0]} + h^{[1]}$, $h^{[0]} = \sum\limits_{\boldsymbol{\alpha}} \epsilon_{\boldsymbol{\alpha}}^{[0]} n_{\boldsymbol{\alpha}}$, $h^{[1]} = \sum \epsilon_\alpha^{[1]} n_\alpha$, $\epsilon_{\boldsymbol{\alpha}}^{[0]} = N_{\boldsymbol{\alpha}}^{-1} \sum\limits_{\alpha\in\boldsymbol{\alpha}} \epsilon_\alpha N_\alpha$ and $\epsilon_\alpha^{[1]} = \epsilon_\alpha - \epsilon_{\boldsymbol{\alpha}}^{[0]}$),

$$
\begin{aligned}
(h^2)_{\text{1-body}} &= \sum \epsilon_\alpha^2 n_\alpha \\
(h^2)_{\text{2-body}} &\Leftrightarrow C_{\alpha\beta\alpha\beta}^J = C_{\alpha\beta} = 2\epsilon_\alpha\epsilon_\beta.
\end{aligned} \tag{5.22}
$$

Eqs. (2.58, 5.22) give the unitary decomposition of the h^2 operator,

$$
\begin{aligned}
(h^2)^{[0]} &= \sum_{\boldsymbol{\alpha}} n_{\boldsymbol{\alpha}} n_{\boldsymbol{\alpha}}^{\times} N_{\boldsymbol{\alpha}\boldsymbol{\alpha}}^{-1} \left\{ \sum_{\alpha\in\boldsymbol{\alpha}} \epsilon_\alpha^2 N_\alpha \right\} \\
(h^2)^{[1]} &= \sum_{\alpha} n_\alpha \left\{ \frac{(N_{\boldsymbol{\alpha}}^{\times} - n_{\boldsymbol{\alpha}})}{(N_{\boldsymbol{\alpha}} - 2)} \left[N_{\boldsymbol{\alpha}}^{-1} \sum_{\alpha'\in\boldsymbol{\alpha}} N_{\alpha'} (\epsilon_\alpha^2 - \epsilon_{\alpha'}^2) \right] \right\} \\
(h^2)^{[2]} &= h^2 - (h^2)^{[0]} - (h^2)^{[1]}
\end{aligned} \tag{5.23}
$$

With $\mathcal{O}_\mu^k$ defined by $\epsilon_{\alpha\beta}^{(k)}$, the one and two-body parts of $\mathcal{O}^\dagger\mathcal{O}$ operator are,

$$
(\mathcal{O}^\dagger\mathcal{O})_{\text{1-body}} = \sum_\beta \left[\left(\sum_\alpha \left\{ \epsilon_{\alpha\beta}^{(k)} \right\}^2 \right) N_\beta^{-1} \right] n_\beta \tag{5.24}
$$

$$
(\mathcal{O}^\dagger\mathcal{O})_{\text{2-body}} = \sum_{k'} \left[\epsilon_{\alpha\beta}^{(k)} \epsilon_{\gamma\delta}^{(k)} \left\{ \begin{array}{ccc} j_\beta & j_\alpha & k \\ j_\delta & j_\gamma & k' \end{array} \right\} \times \right.
$$

$$(-1)^{j_\alpha+j_\beta+j_\gamma+j_\delta+1}\sqrt{(1+\delta_{\beta\gamma})(1+\delta_{\alpha\delta})}\Big]$$

$$\frac{(a_\beta^\dagger a_\gamma^\dagger)_\mu^{k'}}{\sqrt{(1+\delta_{\beta\gamma})}}\frac{\left\{(a_\delta^\dagger a_\alpha^\dagger)_\mu^{k'}\right\}^\dagger}{\sqrt{(1+\delta_{\alpha\delta})}} \tag{5.25}$$

It is easily seen that for the traces under consideration, only the average two-particle matrix elements $C_{\alpha\beta}$ (2.50) of $(\mathcal{O}^\dagger\mathcal{O})_{\text{2-body}}$ will contribute (this is because h^2 operator has only $C_{\alpha\beta}$ part as given in (5.22)). Using (5.25) and the results $\sum_{k'=\text{even}}(2k'+1)\left\{\begin{matrix} j_\alpha & j_\alpha & k \\ j_\alpha & j_\alpha & k'\end{matrix}\right\}=\frac{1}{2}$, $\sum_{k'}(2k'+1)\left\{\begin{matrix} j_\alpha & j_\beta & k \\ j_\alpha & j_\beta & k'\end{matrix}\right\}=1$ for $k\neq 0$ give $C_{\alpha\beta}$ of $\mathcal{O}^\dagger\mathcal{O}$ to be,

$$(\mathcal{O}^\dagger\mathcal{O})_{\text{2-body}} \Leftrightarrow C_{\alpha\beta} = -\left[\left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2+\left\{\epsilon_{\beta\alpha}^{(k)}\right\}^2\right]N_{\alpha\beta}^{-1} \tag{5.26}$$

Eqs. (2.58, 5.25 - 5.27) give the unitary decomposition of the $\mathcal{O}^\dagger\mathcal{O}$ operator,

$$\begin{aligned}
(\mathcal{O}^\dagger\mathcal{O})^{[0]} &= \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}} n_{\boldsymbol{\alpha}} n_{\boldsymbol{\beta}}^{\times} N_{\boldsymbol{\alpha\beta}}^{-1}\times\left[\sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}}\left\{\epsilon_{\beta\alpha}^{(k)}\right\}^2\right]\\
(\mathcal{O}^\dagger\mathcal{O})^{[1]} &= \sum_{\boldsymbol{\alpha},\boldsymbol{\beta};\,\alpha\in\boldsymbol{\alpha},\,\beta\in\boldsymbol{\beta}} n_\alpha\left\{\left(\frac{N_{\boldsymbol{\beta}}-n_{\boldsymbol{\beta}}-\delta_{\boldsymbol{\alpha\beta}}}{N_{\boldsymbol{\beta}}-2\delta_{\boldsymbol{\alpha\beta}}}\right)\right.\\
&\times\left\{(N_\alpha N_{\boldsymbol{\alpha}})^{-1}\sum_{\alpha'\in\boldsymbol{\alpha}}(N_{\alpha'}\left\{\epsilon_{\beta\alpha}^{(k)}\right\}^2-N_\alpha\left\{\epsilon_{\beta\alpha'}^{(k)}\right\}^2)\right\}\\
&-\left(\frac{n_{\boldsymbol{\beta}}-\delta_{\boldsymbol{\alpha\beta}}}{N_{\boldsymbol{\beta}}-2\delta_{\boldsymbol{\alpha\beta}}}\right)\\
&\times\left.\left\{(N_\alpha N_{\boldsymbol{\alpha}})^{-1}\sum_{\alpha'\in\boldsymbol{\alpha}}(N_{\alpha'}\left\{\epsilon_{\alpha\beta}^{(k)}\right\}^2-N_\alpha\left\{\epsilon_{\alpha'\beta}^{(k)}\right\}^2)\right\}\right\}\\
(\mathcal{O}^\dagger\mathcal{O})^{[2]} &= (\mathcal{O}^\dagger\mathcal{O})-(\mathcal{O}^\dagger\mathcal{O})^{[0]}-(\mathcal{O}^\dagger\mathcal{O})^{[1]}
\end{aligned} \tag{5.27}$$

The $\widehat{M}_{PQ}([\mathrm{m}])$ traces with $P+Q\leq 2$ have the following decomposition involving $h^{[0]}$ and $h^{[1]}$,

$$\widehat{M}_{10}([\mathrm{m}]) = \langle\mathcal{O}^\dagger\mathcal{O}h\rangle^{[\mathrm{m}]}=\langle\mathcal{O}^\dagger\mathcal{O}h^{[1]}\rangle^{[\mathrm{m}]}+\langle\mathcal{O}^\dagger\mathcal{O}\rangle^{[\mathrm{m}]}\langle h^{[0]}\rangle^{[\mathrm{m}]}$$

$$
\begin{aligned}
\widehat{M}_{01}([\mathrm{m}]) &= \langle \mathcal{O}^\dagger h \mathcal{O}\rangle^{[\mathrm{m}]} = \langle \mathcal{O}^\dagger \mathcal{O} h^{[1]}\rangle^{[\mathrm{m}]} + \langle \mathcal{O}^\dagger [h^{[1]}, \mathcal{O}]\rangle^{[\mathrm{m}]} + \langle \mathcal{O}^\dagger h^{[0]} \mathcal{O}\rangle^{[\mathrm{m}]} \\
\widehat{M}_{20}([\mathrm{m}]) &= \langle \mathcal{O}^\dagger \mathcal{O} h^2\rangle^{[\mathrm{m}]} = \langle \mathcal{O}^\dagger \mathcal{O} (h^{[1]})^2\rangle^{[\mathrm{m}]} + \langle \mathcal{O}^\dagger \mathcal{O}\rangle^{[\mathrm{m}]} \langle (h^{[0]})^2\rangle^{[\mathrm{m}]} \\
&\quad +2\langle \mathcal{O}^\dagger \mathcal{O} h^{[1]}\rangle^{[\mathrm{m}]} \langle h^{[0]}\rangle^{[\mathrm{m}]} \\
\widehat{M}_{11}([\mathrm{m}]) &= \langle \mathcal{O}^\dagger h \mathcal{O} h\rangle^{[\mathrm{m}]} = \langle \mathcal{O}^\dagger \mathcal{O} (h^{[1]})^2\rangle^{[\mathrm{m}]} + \langle \mathcal{O}^\dagger [h^{[1]}, \mathcal{O}] h^{[1]}\rangle^{[\mathrm{m}]} \\
&\quad +\langle \mathcal{O}^\dagger h^{[0]} \mathcal{O}\rangle^{[\mathrm{m}]} \langle h^{[0]}\rangle^{[\mathrm{m}]} + \langle \mathcal{O}^\dagger [h^{[1]}, \mathcal{O}]\rangle^{[\mathrm{m}]} \langle h^{[0]}\rangle^{[\mathrm{m}]} \\
&\quad +\langle \mathcal{O}^\dagger [h^{[0]}, \mathcal{O}] h^{[1]}\rangle^{[\mathrm{m}]} + 2\langle \mathcal{O}^\dagger \mathcal{O} h^{[1]}\rangle^{[\mathrm{m}]} \langle h^{[0]}\rangle^{[\mathrm{m}]} \\
\widehat{M}_{02}([\mathrm{m}]) &= \langle \mathcal{O}^\dagger h^2 \mathcal{O}\rangle^{[\mathrm{m}]} = \langle \mathcal{O}^\dagger \mathcal{O} (h^{[1]})^2\rangle^{[\mathrm{m}]} + 2\langle \mathcal{O}^\dagger [h^{[1]}, \mathcal{O}] h^{[1]}\rangle^{[\mathrm{m}]} \\
&\quad +\langle \mathcal{O}^\dagger [h^{[1]}, [h^{[1]}, \mathcal{O}]]\rangle^{[\mathrm{m}]} + \langle \mathcal{O}^\dagger (h^{[0]})^2 \mathcal{O}\rangle^{[\mathrm{m}]} \\
&\quad +2\{\langle \mathcal{O}^\dagger [h^{[0]}, \mathcal{O}] h^{[1]}\rangle^{[\mathrm{m}]} + \langle \mathcal{O}^\dagger \mathcal{O} h^{[1]}\rangle^{[\mathrm{m}]} \langle h^{[0]}\rangle^{[\mathrm{m}]}\} \\
&\quad +2\langle \mathcal{O}^\dagger h^{[0]} [h^{[1]}, \mathcal{O}]\rangle^{[\mathrm{m}]} \qquad (5.28)
\end{aligned}
$$

and therefore the basic traces needed for evaluating $\widehat{M}_{PQ}$ with $P+Q \leq 2$ are, $\langle \mathcal{O}^\dagger \mathcal{O}\rangle^{[\mathrm{m}]}$, $\langle \mathcal{O}^\dagger (h^{[0]})^P \mathcal{O}\rangle^{[\mathrm{m}]}$, $\langle \mathcal{O}^\dagger \mathcal{O} h^{[1]}\rangle^{[\mathrm{m}]}$, $\langle \mathcal{O}^\dagger [h^{[1]}, \mathcal{O}]\rangle^{[\mathrm{m}]}$, $\langle \mathcal{O}^\dagger [h^{[0]}, \mathcal{O}]\rangle^{[\mathrm{m}]}$, $\langle \mathcal{O}^\dagger \mathcal{O} (h^{[1]})^2\rangle^{[\mathrm{m}]}$, $\langle \mathcal{O}^\dagger [h^{[1]}, \mathcal{O}] h^{[1]}\rangle^{[\mathrm{m}]}$, $\langle \mathcal{O}^\dagger [h^{[0]}, \mathcal{O}] h^{[1]}\rangle^{[\mathrm{m}]}$, $\langle \mathcal{O}^\dagger [h^{[1]}, [h^{[1]}, \mathcal{O}]]\rangle^{[\mathrm{m}]}$, $\langle \mathcal{O}^\dagger h^{[0]} [h^{[1]}, \mathcal{O}]\rangle^{[\mathrm{m}]}$ and $\langle (h^{[0]})^P\rangle^{[\mathrm{m}]}$. Propagation equations for these eleven basic traces are derived using the unitary decompositions given by (5.23, 5.27).

For $\langle \mathcal{O}^\dagger \mathcal{O}\rangle^{[\mathrm{m}]}$ trace, only $(\mathcal{O}^\dagger \mathcal{O})^{[0]}$ contributes (due to invariance properties of traces) and then the trace propagation formula is,

$$
\langle \mathcal{O}^\dagger \mathcal{O}\rangle^{[\mathrm{m}]} = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}} m_{\boldsymbol{\alpha}} m_{\boldsymbol{\beta}}^{\times} N_{\boldsymbol{\alpha}\boldsymbol{\beta}}^{-1} \left\{ \sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}} \left\{\epsilon_{\beta\alpha}^{(k)}\right\}^2 \right\} \qquad (5.29)
$$

The decomposition of $\langle \mathcal{O}^\dagger \mathcal{O}\rangle^{[\mathrm{m}]}$ into partial traces involving intermediate $[\mathrm{m}']$ configurations is immediate; $[\mathrm{m}'] = [\mathrm{m}] \times \left(1_{\boldsymbol{\beta}}^\dagger 1_{\boldsymbol{\alpha}}\right)$. Therefore, using (5.29), the propagation formula for $\langle \mathcal{O}^\dagger (h^{[0]})^P \mathcal{O}\rangle^{[m]}$ is given by,

$$\langle \mathcal{O}^\dagger (h^{[0]})^P \mathcal{O}\rangle^{[m]} = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}} \left\{ m_{\boldsymbol{\alpha}} m^{\times}_{\boldsymbol{\beta}} N^{-1}_{\boldsymbol{\alpha\beta}} \times \sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\beta\alpha}\right\}^2 \right\} \times \left\{ \sum_{\boldsymbol{\tau}} \epsilon^{[0]}_{\boldsymbol{\tau}} m'_{\boldsymbol{\tau}} \right\}^P \delta\left([m'], [m] \times (1^\dagger_{\boldsymbol{\beta}} 1_{\boldsymbol{\alpha}}) \right) \quad (5.30)$$

In order to derive the formula for $\langle \mathcal{O}^\dagger \mathcal{O} h^{[1]}\rangle^{[m]}$, it should be recognized that only $(\mathcal{O}^\dagger \mathcal{O})^{[1]}$ part of $\mathcal{O}^\dagger \mathcal{O}$ contributes to the trace (as $[\boldsymbol{\nu}] \times [1]$ yields $[0]$ only with $[\boldsymbol{\nu}] = [1]$). Using $(\mathcal{O}^\dagger \mathcal{O})^{[1]})$ given in (5.27) and $h^{[1]}$ given above (5.22) together with (5.16) immediately produces,

$$\langle \mathcal{O}^\dagger \mathcal{O} h^{[1]}\rangle^{[m]} = \sum_{\boldsymbol{\alpha\beta}} \left\{ \left[m_{\boldsymbol{\alpha}} m^{\times}_{\boldsymbol{\alpha\beta}} N^{-1}_{\boldsymbol{\alpha\alpha\beta}} \right] \sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\beta\alpha}\right\}^2 \epsilon^{[1]}_{\alpha} - \left[m_{\boldsymbol{\alpha\beta}} m^{\times}_{\boldsymbol{\alpha}} N^{-1}_{\boldsymbol{\alpha\alpha\beta}} \right] \times \sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\alpha\beta}\right\}^2 \epsilon^{[1]}_{\alpha} \right\} \quad (5.31)$$

It is interesting to note that the scalar propagation formula (5.16) for $\langle \mathcal{O}^\dagger \mathcal{O} \widetilde{h}\rangle^m$ symbolically translates into (5.31). This rather important and interesting connection between scalar traces and unitary configurations traces is not yet fully understood. Using the result that $[h^{[1]}, \mathcal{O}] \doteq \mathcal{O}'$ with $\mathcal{O}'$ defined by $\left\{\epsilon^{(k)}_{\alpha\beta}\right\}'$s where $[h^{[1]}, \mathcal{O}] = \mathcal{O}' \Rightarrow \left\{\epsilon^{(k)}_{\alpha\beta}\right\}' = \epsilon^{(k)}_{\alpha\beta}(\epsilon^{[1]}_{\alpha} - \epsilon^{[1]}_{\beta})$ and (5.29), give directly the formulas (changing $\left\{\epsilon^{(k)}_{\beta\alpha}\right\}^2$ in (5.29) into $\left\{\epsilon^{(k)}_{\beta\alpha}\right\}\left\{\epsilon^{(k)}_{\beta\alpha}\right\}'$) for $\langle \mathcal{O}^\dagger [h^{[1]}, \mathcal{O}]\rangle^{[m]}$ and $\langle \mathcal{O}^\dagger [h^{[0]}, \mathcal{O}]\rangle^{[m]}$,

$$\langle \mathcal{O}^\dagger [h^{[1]}, \mathcal{O}]\rangle^{[m]} = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}} m_{\boldsymbol{\alpha}} m^{\times}_{\boldsymbol{\beta}} N^{-1}_{\boldsymbol{\alpha\beta}} \left\{ \sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\beta\alpha}\right\}^2 (\epsilon^{[1]}_{\beta} - \epsilon^{[1]}_{\alpha}) \right\} \quad (5.32)$$

$$\langle \mathcal{O}^\dagger [h^{[0]}, \mathcal{O}]\rangle^{[m]} = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}} m_{\boldsymbol{\alpha}} m^{\times}_{\boldsymbol{\beta}} N^{-1}_{\boldsymbol{\alpha\beta}} \left\{ \sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\beta\alpha}\right\}^2 (\epsilon^{[0]}_{\boldsymbol{\beta}} - \epsilon^{[0]}_{\boldsymbol{\alpha}}) \right\} \quad (5.33)$$

In order to derive the expression for $\langle \mathcal{O}^\dagger \mathcal{O}(h^{[1]})^2 \rangle^{[m]}$, the SPE and TBME of $\mathcal{O}^\dagger\mathcal{O}$ and $(h^{[1]})^2$ operators as given by (5.22) and (5.24 - 5.26) and the corresponding unitary decompositions given by (5.23) and (5.27) respectively are used. The trace orthogonality equation (3.13) and the trace propagation equations (2.71, 2.72) give,

$$
\begin{aligned}
\langle \mathcal{O}^\dagger \mathcal{O}(h^{[1]})^2 \rangle^{[m]} &= \left[\sum_{\boldsymbol{\alpha}}[\mathcal{E}_{\boldsymbol{\alpha}}(\{h^{[1]}\}^2)]m_{\boldsymbol{\alpha}} + \sum_{\boldsymbol{\alpha}\geq\boldsymbol{\beta}}[C_{\boldsymbol{\alpha\beta}}(\{h^{[1]}\}^2)]m_{\boldsymbol{\alpha\beta}}\right] \\
&\times \left[\sum_{\boldsymbol{\alpha}}[\mathcal{E}_{\boldsymbol{\alpha}}(\mathcal{O}^\dagger\mathcal{O})]m_{\boldsymbol{\alpha}} + \sum_{\boldsymbol{\alpha}\geq\boldsymbol{\beta}}[C_{\boldsymbol{\alpha\beta}}(\mathcal{O}^\dagger\mathcal{O})]m_{\boldsymbol{\alpha\beta}}\right] \\
&+ \sum_{\boldsymbol{\alpha}} m_{\boldsymbol{\alpha}} m^{\times}_{\boldsymbol{\alpha}} N^{-1}_{\boldsymbol{\alpha\alpha}} \left[\sum_{\alpha\in\boldsymbol{\alpha}} N_\alpha \times \right. \\
&\left\{[\mathcal{E}^{[1]}_\alpha\{(h^{[1]})^2\}] + \sum_{\boldsymbol{\beta}}(m_{\boldsymbol{\beta}} - \delta_{\boldsymbol{\alpha\beta}})[\mathcal{E}^{[1];\boldsymbol{\beta}}_\alpha\{(h^{[1]})^2\}]\right\} \\
&\times \left.\left\{[\mathcal{E}^{[1]}_\alpha(\mathcal{O}^\dagger\mathcal{O})] + \sum_{\beta\in\boldsymbol{\beta}}(m_{\boldsymbol{\beta}} - \delta_{\boldsymbol{\alpha\beta}})[\mathcal{E}^{[1];\boldsymbol{\beta}}_\alpha(\mathcal{O}^\dagger\mathcal{O})]\right\}\right] \\
&+ \sum_{\boldsymbol{\alpha}\geq\boldsymbol{\beta}} m_{\boldsymbol{\alpha\beta}} m^{\times}_{\boldsymbol{\alpha\beta}} N^{-1}_{\boldsymbol{\alpha\beta\alpha\beta}}
\end{aligned}
$$

$$
\times \left[\left\{\sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}} [C_{\alpha\beta}(\{h^1\}^2)][C_{\alpha\beta}(\mathcal{O}^\dagger\mathcal{O})]N_{\alpha\beta}(1+\delta_{\alpha\beta})\right\}(1+\delta_{\boldsymbol{\alpha\beta}})^{-1}\right]. \quad (5.34)
$$

Trace propagation formulas for $\langle \mathcal{O}^\dagger[h^{[1]},\mathcal{O}]h^{[1]}\rangle\rangle^{[m]}$ and $\langle \mathcal{O}^\dagger[h^{[0]},\mathcal{O}]h^{[1]}\rangle\rangle^{[m]}$ follow from the use of (5.31) and the $\mathcal{O}'$ operator defined above (5.32),

$$
\begin{aligned}
\langle \mathcal{O}^\dagger[h^{[1]},\mathcal{O}]h^{[1]}\rangle\rangle^{[m]} &= \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}} \left\{\left[m_{\boldsymbol{\alpha}} m^{\times}_{\boldsymbol{\alpha\beta}} N^{-1}_{\boldsymbol{\alpha\alpha\beta}} \sum_{\alpha\in\boldsymbol{\alpha},\,\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\beta\alpha}\right\}^2 \epsilon^{[1]}_\alpha(\epsilon^{[1]}_\beta - \epsilon^{[1]}_\alpha)\right]\right. \\
&+ \left.\left[m_{\boldsymbol{\alpha\beta}} m^{\times}_{\boldsymbol{\alpha}} N^{-1}_{\boldsymbol{\alpha\alpha\beta}} \sum_{\alpha\in\boldsymbol{\alpha},\,\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\alpha\beta}\right\}^2 \epsilon^{[1]}_\alpha(\epsilon^{[1]}_\beta - \epsilon^{[1]}_\alpha)\right]\right\}
\end{aligned}
$$

(5.35)

$$\langle \mathcal{O}^\dagger [h^{[0]}, \mathcal{O}] h^{[1]} \rangle^{[\mathrm{m}]} = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}} \left\{ \left[m_{\boldsymbol{\alpha}} m^{\times}_{\boldsymbol{\alpha\beta}} N^{-1}_{\boldsymbol{\alpha\alpha\beta}} \sum_{\alpha\in\boldsymbol{\alpha},\,\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\beta\alpha}\right\}^2 \epsilon^{[1]}_{\alpha} (\epsilon^{[0]}_{\boldsymbol{\beta}} - \epsilon^{[0]}_{\boldsymbol{\alpha}}) \right] \right.$$

$$\left. + \left[m_{\boldsymbol{\alpha\beta}} m^{\times}_{\boldsymbol{\alpha}} N^{-1}_{\boldsymbol{\alpha\alpha\beta}} \sum_{\alpha\in\boldsymbol{\alpha},\,\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\alpha\beta}\right\}^2 \epsilon^{[1]}_{\alpha} (\epsilon^{[0]}_{\boldsymbol{\beta}} - \epsilon^{[0]}_{\boldsymbol{\alpha}}) \right] \right\} \tag{5.36}$$

The expression for $\langle \mathcal{O}^\dagger [h^{[1]}, [h^{[1]}, \mathcal{O}]] \rangle^{[\mathrm{m}]}$ is obtained by recognizing that $[h^{[1]}, [h^{[1]}, \mathcal{O}]] \Rightarrow [h^{[1]}, \mathcal{O}'] \Rightarrow \mathcal{O}''$ defined by $\left(\epsilon^{(k)}_{\alpha\beta}\right)'' = \epsilon^{(k)}_{\alpha\beta}\left(\epsilon^{[1]}_{\alpha} - \epsilon^{[1]}_{\beta}\right)^2$ and then using (5.29),

$$\langle \mathcal{O}^\dagger [h^{[1]}, [h^{[1]}, \mathcal{O}]] \rangle^{[\mathrm{m}]} = \sum_{\boldsymbol{\alpha\beta}} \left\{ m_{\boldsymbol{\alpha}} m^{\times}_{\boldsymbol{\beta}} N^{-1}_{\boldsymbol{\alpha\beta}} \right\} \sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\beta\alpha}\right\}^2 \{\epsilon^{[1]}_{\beta} - \epsilon^{[1]}_{\alpha}\}^2 \tag{5.37}$$

The expression for $\langle \mathcal{O}^\dagger h^{[0]} [h^{[1]}, \mathcal{O}] \rangle^{[\mathrm{m}]}$ follows easily from the $\left(\epsilon^{(k)}_{\alpha\beta}\right)'$ of $[h^{[1]}, \mathcal{O}]$ and (5.30),

$$\langle \mathcal{O}^\dagger h^{[0]} [h^{[1]}, \mathcal{O}] \rangle^{[\mathrm{m}]} = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}} \left\{ m_{\boldsymbol{\alpha}} m^{\times}_{\boldsymbol{\beta}} N^{-1}_{\boldsymbol{\alpha\beta}} \right\} \left[\sum_{\alpha\in\boldsymbol{\alpha},\beta\in\boldsymbol{\beta}} \left\{\epsilon^{(k)}_{\beta\alpha}\right\}^2 (\epsilon^{[1]}_{\beta} - \epsilon^{[1]}_{\alpha}) \right]$$
$$\times \left[\left\{ \sum_{\boldsymbol{\tau}} \epsilon^{[0]}_{\boldsymbol{\tau}} m'_{\boldsymbol{\tau}} \right\} \delta\left([\mathrm{m}'], [\mathrm{m}] \times \left(1^\dagger_{\boldsymbol{\beta}} 1_{\boldsymbol{\alpha}} \right) \right) \right]. \tag{5.38}$$

Finally, the expression for $\langle (h^{[0]})^P \rangle^{[\mathrm{m}]}$ is,

$$\langle (h^{[0]})^P \rangle^{[\mathrm{m}]} = \left\{ \sum_{\boldsymbol{\alpha}} m_{\boldsymbol{\alpha}} \epsilon^{[0]}_{\boldsymbol{\alpha}} \right\}^P \tag{5.39}$$

It should be mentioned that the formulas (5.29 - 5.39) are verified numerically by using (5.12) and (5.10).

5.7.2 pn systems

For pn one-body transition operators that belong to categories [B], [C] or [D] (5.2) and with pn unitary configurations ([m] $\rightarrow$ [$\mathbf{m_p}$, $\mathbf{m_n}$]), the results in

(5.29 - 5.39) will apply when the conventions given in Sect. 3.1.5 are used. It should be stressed that the order of the indices in $\epsilon^{(k)}_{\alpha\beta}$ should be kept as they are given in Eqs. 5.22 - 5.39 and without this, the results for operators belonging to categories [C] and [D] will be wrong (the phase relation $\epsilon^{(k)}_{\alpha\beta} = (-1)^{j_\alpha - j_\beta} \epsilon^{(k)}_{\beta\alpha}$ is valid only when α, $\beta \in$ p or n; its extension to the case with $\alpha \in$ p, $\beta \in$ n or $\alpha \in$ n $\beta \in$ p is immediate). For pn one-body transition operators that belong to categories [B], [C] or [D] (5.2) and with pn unitary configurations ([m] $\rightarrow$ [$\mathbf{m_p}$, $\mathbf{m_n}$]), the results in (5.29 - 5.39) will apply when the conventions given in Sect. 3.1.5 are used. As an example the TBME for $GT(\beta^{\pm})$ operator can be written down using (5.25),

$$
\begin{aligned}
V^{k'}_{\alpha_p\beta_n\gamma_p\delta_n}(GT(\beta^-)) &= -\epsilon^{(1)}_{\alpha_p\delta_n}\epsilon^{(1)}_{\gamma_p\beta_n}\left\{\begin{array}{ccc} j_\beta & j_\gamma & k=1 \\ j_\delta & j_\alpha & k' \end{array}\right\} \\
V^{k'}_{\alpha_n\beta_p\gamma_n\delta_p}(GT(\beta^-)) &= (-1)^{j_\alpha+j_\beta+j_\gamma+j_\delta+1}\epsilon^{(1)}_{\beta_p\gamma_n}\epsilon^{(1)}_{\delta_p\alpha_n}\left\{\begin{array}{ccc} j_\alpha & j_\delta & k=1 \\ j_\gamma & j_\beta & k' \end{array}\right\}
\end{aligned}
\tag{5.40}
$$

The phase relation

$$
\epsilon^{(1)}_{\alpha_p\delta_n} = (-1)^{j_\alpha - j_\delta}\epsilon_{\delta_p\alpha_n} \tag{5.41}
$$

immediately shows that $V^{k'}_{\alpha_n\beta_p\gamma_n\delta_p}(GT(\beta^-)) = V^{k'}_{\alpha_p\beta_n\gamma_p\delta_n}(GT(\beta^-))$ as required. The TBME for $(GT(\beta^+))$ operator follow easily from the second equation in (5.40),

$$
V^{k'}_{\alpha_p\beta_n\gamma_p\delta_n}(GT(\beta^+)) = (-1)^{j_\alpha+j_\beta+j_\gamma+j_\delta+1}\epsilon^{(1)}_{\beta_n\gamma_p}\epsilon^{(1)}_{\delta_n\alpha_p}\left\{\begin{array}{ccc} j_\alpha & j_\delta & k=1 \\ j_\gamma & j_\beta & k' \end{array}\right\} \tag{5.42}
$$

Finally note that $\epsilon^{(1)}_{\alpha_n\beta_p}$ also satisfies the phase relation (5.41); $\epsilon^{(1)}_{\alpha_n\beta_p} = (-1)^{j_\alpha - j_\beta}\epsilon^{(1)}_{\beta_n\alpha_p}$.

5.7.3 Partial $\mathbf{M}_{PQ}([\mathrm{m}],[\mathrm{m}'])$ moments

Given the initial configuration $[\mathrm{m}]$, the $\epsilon^{(k)}_{\alpha\beta}$ terms appearing in (5.29 - 5.39) immediately define the projection operator $\mathbf{P}([\mathrm{m}'])$ in (5.12) or in other words uniquely the $[\mathrm{m}']$ configuration; $[\mathrm{m}'] = [\mathrm{m}] \times \left(1^{\dagger}_{\alpha} 1_{\beta}\right)$. It is easy to obtain $\mathbf{M}_{PQ}([\mathrm{m},\mathrm{m}'])$ moments by calculating $\widehat{M}_{PQ}([\mathrm{m}])$ moments for different $\epsilon^{(k)}_{\alpha\beta}$ terms separately. We will illustrate this with an example. Let us consider $GT(\beta^-)$ operator in a 7-orbit shell model space consisting of ds and fp-shells with ds-shell as one unitary orbit and fp-shell as another unitary orbit. Then there are two unitary orbits for protons and two for neutrons labelled as $\boldsymbol{\alpha} = 1,2,3$ and 4 respectively. From the definition of $\epsilon^{(k)}_{\alpha\beta}$ given in (5.3), it is clear that the partial moments are non-zero only for $S = S'$. In other words, for non-zero partial moments both α(p) and β(n) should belong to ds-shell or both should belong to fp-shell in this particular example. Therefore for a unitary configuration $[m_1, m_2, m_3, m_4]$, where $m_1 \in \boldsymbol{\alpha} = 1$, $m_2 \in \boldsymbol{\alpha} = 2$, $m_3 \in \boldsymbol{\alpha} = 3$ and $m_4 \in \boldsymbol{\alpha} = 4$, the possible final configurations are $[m_1{+}1, m_2, m_3{-}1, m_4]$ and $[m_1, m_2{+}1, m_3, m_4{-}1]$ where for the first configuration $\epsilon^{(k)}_{\alpha\beta}$ with $\alpha \in \boldsymbol{\alpha} = 1$ and $\beta \in \boldsymbol{\beta} = 3$ will contribute while for the second configuration $\epsilon^{(k)}_{\alpha\beta}$ with $\alpha \in \boldsymbol{\alpha} = 2$ and $\beta \in \boldsymbol{\beta} = 4$ will contribute. Therefore by putting $\epsilon^{(k)}_{\alpha\beta} = 0$ for $\alpha \in \boldsymbol{\alpha} = 2$, $\beta \in \boldsymbol{\beta} = 4$, gives $\widehat{M}_{PQ}([\mathrm{m}])/\widehat{M}_{00}([\mathrm{m}]) = \mathbf{M}_{PQ}([m_1, m_2, m_3, m_4], [m_1 + 1, m_2, m_3 - 1, m_4])/\ \mathbf{M}_{00}([m_1, m_2, m_3, m_4], [m_1 + 1, m_2, m_3 - 1, m_4])$ and similarly by putting $\epsilon^{(k)}_{\alpha\beta} = 0$ for $\alpha \in \boldsymbol{\alpha} = 1$, $\beta \in \boldsymbol{\beta} = 3$, gives $\widehat{M}_{PQ}\ ([m_1, m_2, m_3, m_4])/\widehat{M}_{00}\ ([m_1, m_2, m_3, m_4]) = \mathbf{M}_{PQ}([m_1, m_2, m_3, m_4], [m_1, m_2{+}1, m_3, m_4{-}1])/\mathbf{M}_{00}([m_1, m_2, m_3, m_4], [m_1, m_2{+}1, m_3, m_4{-}1])$. With the same numerical example considered in Sect. 5.5 (i.e. $m_p = 4, m_n = 6 \rightarrow m_p = 5, m_n = 5$), and using the above equality between $\widehat{M}_{PQ}([\mathrm{m}])$ and

$\mathbf{M}_{PQ}([\mathbf{m}],[\mathbf{m}'])$ it is explicitly verified that (5.29 - 5.39) reproduce exactly the numbers given by (5.12, 5.10, 5.3).

5.8 Test of moment method for constructing $\mathbf{I}^h_{\mathcal{O}(GT)}$

The results of Sects. 5.4 and 5.5 allow one to construct the exact NIP strength density $\mathbf{I}^h_{\mathcal{O}}$ for one-body transition operators and the results of Sect. 5.7 via superposition of partial strength densities $\mathbf{I}^{h;[\mathbf{m}],[\mathbf{m}']}_{\mathcal{O}}$ represented by bivariate Gaussians with their five parameters calculated directly (without recourse to spherical configurations) in terms of bivariate moments $\mathbf{M}_{PQ}([\mathbf{m}],[\mathbf{m}'])$. In order to test the moment method (which is rapid and produces a smooth density) in *large spaces*, a numerical test is carried out using $GT(\beta^-)$ operator. Using the same s.p. orbits and SPE as given in the numerical example of Sect. 5.5 and the unitary orbits to be $[1d_{5/2}]$, $[2s_{1/2}, 1d_{3/2}]$, $[f_{7/2}]$ and $[2p_{3/2}, 1f_{5/2}, 2p_{1/2}]$ with $\alpha = 1,2,3$ and 4 respectively for protons and similarly for neutrons with $\alpha = 5,6,7$ and 8 respectively, the NIP strength density is calculated for $(m_p, m_n) = (4,6) \Rightarrow (m'_p, m'_n) = (5,5)$ with $S = 0,1$ and 2 (note that $s = 0$ for ds and $s = 1$ for fp-shell orbits). In this example there are 385 (35 $S = 0$, 116 $S = 1$ and 234 $S = 2$) unitary configurations against 5748 spherical configurations. The exact density is calculated using the formalism given in Sect. 5.4; this is denoted by $\mathbf{I}^h_{\mathcal{O}(GT);Ex}$. The strength density as superposition of bivariate Edgeworth corrected Gaussian representation (2.21) for the partial $\mathbf{I}^{h;[\mathbf{m}],[\mathbf{m}']}_{\mathcal{O}(GT)}$ densities is constructed using the results in Sects. 5.4, 5.5 (i.e. using the exact density to calculate k_{rs} with $r + s = 3,4$); the resulting

Figure 5.1

NIP strength densities $\mathbf{I}^h_{\mathcal{O}(GT)}$ and their S-decompositions for $GT(\beta^-)$ transition operator. The densities $\mathbf{I}^h_{\mathcal{O}(GT)}$ are in MeV^{-2} units. Shown in the figures are $\ell og(\mathbf{I}^h_{\mathcal{O}(GT)}(E,E'))$ for E and E' upto 40 MeV:

(a) $S=0$ exact density $\mathbf{I}^{h,S=0}_{\mathcal{O}(GT(\beta^-));Ex}$,

(b) $\mathbf{I}^{h,S=0}_{\mathcal{O}(GT(\beta^-));\mathcal{G}}$,

(c) $S=1$ exact density $\mathbf{I}^{h,S=1}_{\mathcal{O}(GT(\beta^-));Ex}$,

(d) $\mathbf{I}^{h,S=1}_{\mathcal{O}(GT(\beta^-));\mathcal{G}}$,

(e) $S=2$ exact density $\mathbf{I}^{h,S=2}_{\mathcal{O}(GT(\beta^-));Ex}$,

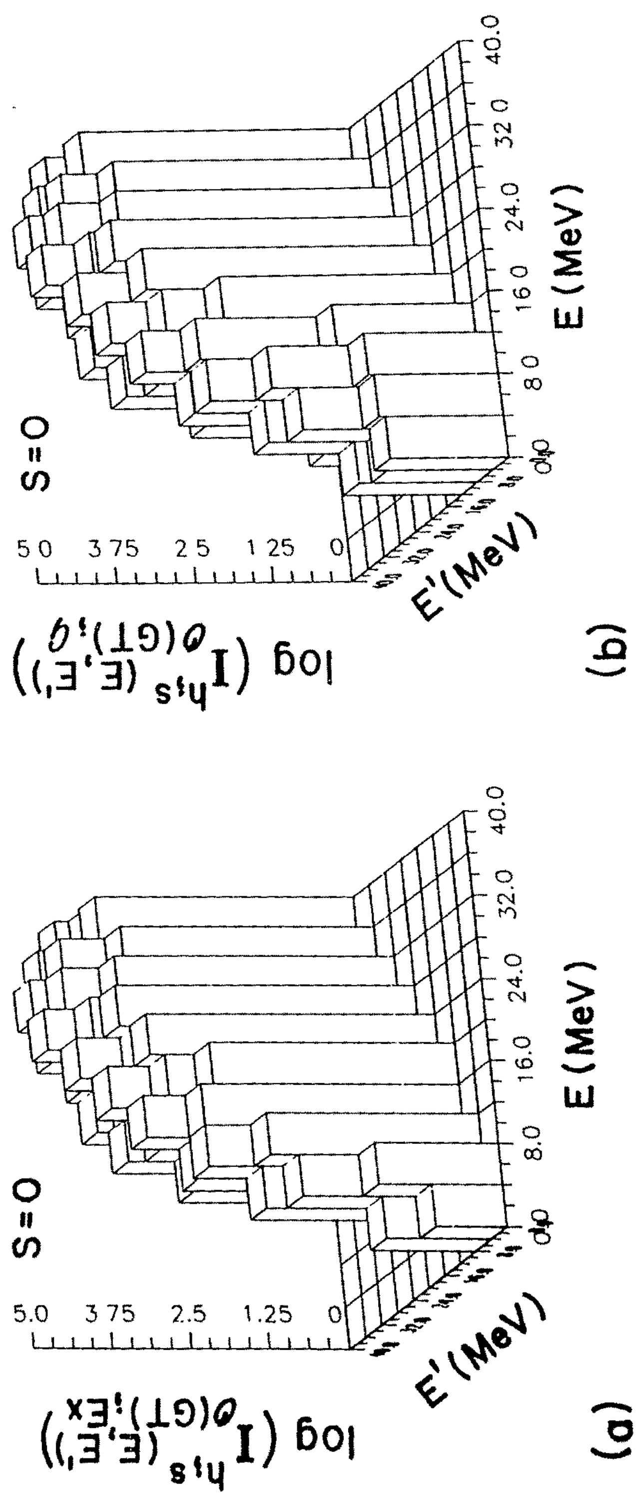
(f) $\mathbf{I}^{h,S=2}_{\mathcal{O}(GT(\beta^-));\mathcal{G}}$,

(g) Exact total ($S=0\oplus 1\oplus 2$) density, $\mathbf{I}^{h}_{\mathcal{O}(GT(\beta^-));Ex}$,

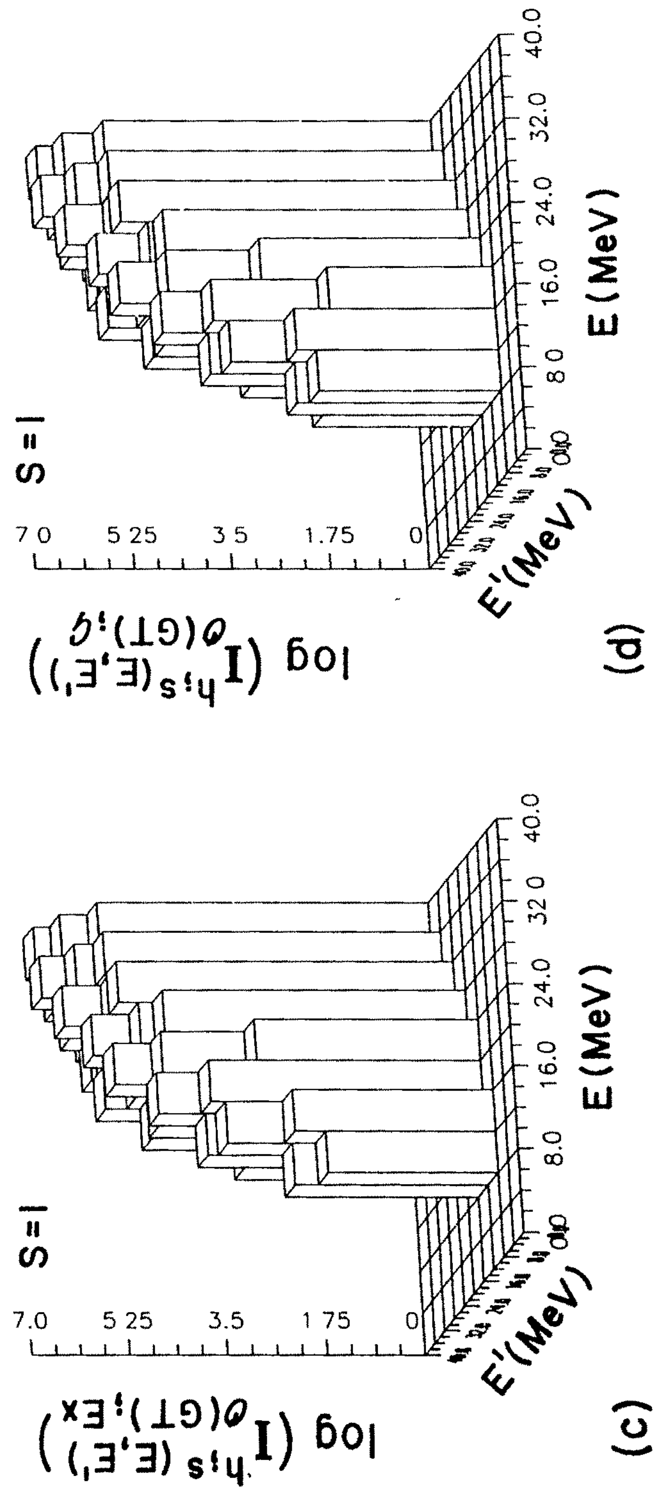
(h) Total ($S=0\oplus 1\oplus 2$) density $\mathbf{I}^{h}_{\mathcal{O}(GT(\beta^-));\mathcal{G}}$,

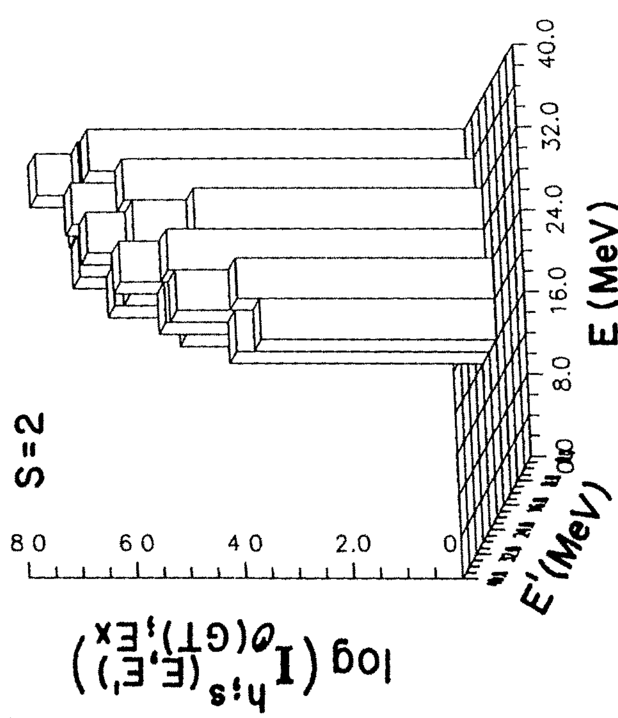
(i) Total ($S=0\oplus 1\oplus 2$) density $\mathbf{I}^{h}_{\mathcal{O}(GT(\beta^-));Ed}$.

See text for the definitions of the bivariate densities $\mathbf{I}^h_{\mathcal{O}(GT);\mathcal{G}}$ and $\mathbf{I}^h_{\mathcal{O}(GT);Ed}$ and also for all the calculational details.

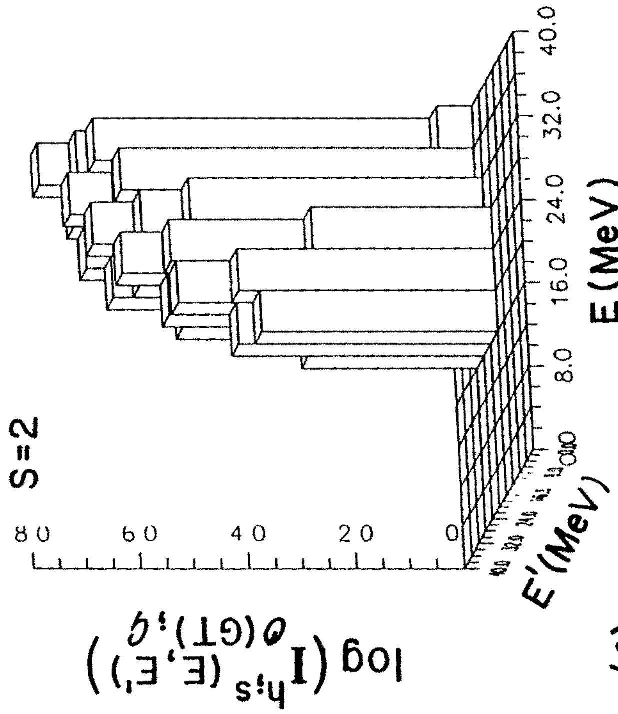


S=0
E (MeV)
E'(MeV)
5.0
3.75
2.5
1.25
0
8.0
16.0
24.0
32.0
40.0
(a)
(b)

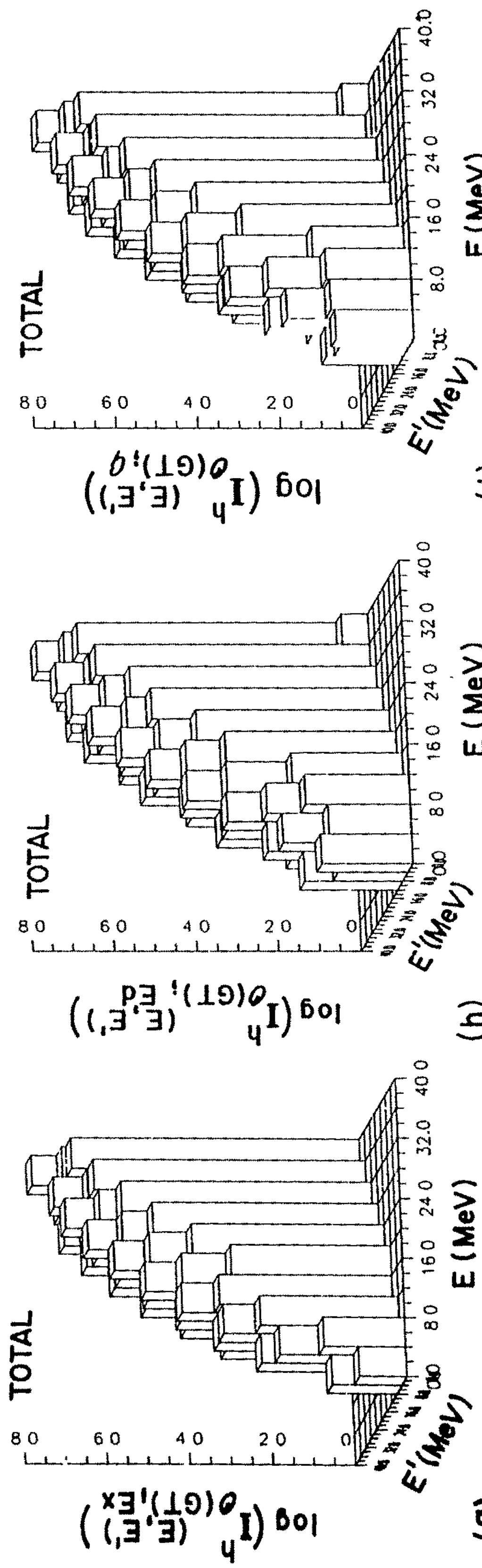

S=1
7.0
5.25
3.5
1.75
0
E(MeV)
E'(MeV)
(d)
(c)


S=2
80
60
40
2.0
0
E'(MeV)
0.0
8.0
16.0
24.0
32.0
40.0
E (MeV)

(e)


S=2
80
60
40
20
0
E'(MeV)
0.0
8.0
16.0
24.0
32.0
40.0
E (MeV)

(f)



TOTAL
E (MeV)
E'(MeV)
(g)
(h)
(i)

density is denoted by $\mathbf{I}^h_{\mathcal{O}(GT);Ed}$. The strength density as a superposition of bivariate Gaussian forms for $\mathbf{I}^{h;[\mathbf{m}],[\mathbf{m}']}_{\mathcal{O}(GT)}$ densities is constructed using the results of Sect. 5.7; the resulting density is denoted by $\mathbf{I}^h_{\mathcal{O}(GT);\mathcal{G}}$. In the construction of bivariate Gaussian or Edgeworth form, care has been taken to treat the singularities properly (this situation arises for example if correlation coefficient is unity). Choosing a bin size of 4 MeV $\times$ 4 MeV (this choice of the bin size follows from [Dr-77b]), histograms for $\mathbf{I}^h_{\mathcal{O}(GT);Ex}$, $\mathbf{I}^h_{\mathcal{O}(GT);Ed}$ and $\mathbf{I}^h_{\mathcal{O}(GT);\mathcal{G}}$ and their S - decompositions are constructed and some of the results are shown in Figs. 5.1a - 5.1i. It is clear from the figures that the bivariate Gaussian representation of $\mathbf{I}^{h;[\mathbf{m}],[\mathbf{m}']}_{\mathcal{O}(GT)}$ describes the exact results for total density as well as their S - decompositions. It should be added that in the cases when k_{rs} with $r + s = 3, 4$ are needed (i.e. departures from bivariate Gaussian are important), these higher order cumulants can be calculated using (5.10) for a random sampling of $([\mathbf{m}], [\mathbf{m}'])$ configurations and use them in determining the cumulants for all the $([\mathbf{m}], [\mathbf{m}'])$ configurations (there are various ways one can divide the unitary configurations into classes or groups). Alternatively it is also possible to use the estimates for k_{rs} as given by the scalar trace formulas of Sect. 5.6 and discussed for example following (5.20). Finally it should be mentioned that agreements similar to what are shown in Figs. 5.1a - 5.1i are also obtained for $GT(\beta^+)$ operator.

5.9 Summary

Complete formalism for constructing NIP strength densities, which enter into IP strength densities as one of the convolution factors, and their unitary orbit decompositions is worked out for one-body transition operators and tested in a large space example. The formalism given in Sects. 5.4 - 5.7 together with the spreading densities generated by interactions, is employed in the next chapter to give a method for calculating β-decay rates for massive presupernova stars.