Chapter 2

Some Mathematical Aspects of Spectral Averaging Theory

2.1 Preview

In spectral averaging theory, as briefly described in Chapter 1, one derives and applies smoothed forms for state, expectation value and strength densities. In Sect. 2.2 some important properties of univariate (that characterize for example state and expectation value densities) and bivariate (that characterize for example strength densities) distributions, well known to statisticians [Ke-69], are given. The definitions, in terms of a given hamiltonian H and m-particle spectroscopic spaces, of state, expectation value and strength densities, their moments and the corresponding CLT results are given in Sect. 2.3. Spherical and unitary configurations partitioning of m-particle scalar spaces and the corresponding decompositions of various densities into partial densities, which play a special role in SAT-LSS are introduced in Sect. 2.4. An important ingredient of spectral theory which plays a vital role in the result presented in Chapters 3 - 6 and also which is essential for deriving trace propagation

formulas that enable one to calculate moments is the unitary group (tensorial) decomposition of operators and this is briefly described with examples in Sect. 2.5. Finally the basic elements of trace propagation and some important trace propagation formulas are given in Sect. 2.6. The results given in Sects. 2.3 - 2.6 are limited to those that are essential for following Chapters 3 - 6 and it should be mentioned that all the results in this chapter are borrowed from available literature.

2.2 Statistical distributions

2.2.1 Univariate distributions

Given a univariate probability density function (or simply density) $\rho(x)$, at the outset it is assumed that, it is positive definite and normalized to unity,

$$\int_{-\infty}^{+\infty} \rho(x)dx = 1 \ ,$$

$$\rho(x) > 0 \, ; \ -\infty \leq x \leq +\infty \tag{2.1}$$

The characteristic function $\phi(t)$ which is the Fourier transform of $\rho(x)$, define the moments M_r of $\rho(x)$,

$$\begin{aligned} \phi(t) &= \int_{-\infty}^{+\infty} exp(itx)\rho(x)dx = \sum_r \frac{(it)^r}{r!} M_r \\ M_r &= \int_{-\infty}^{+\infty} \rho(x)x^r dx. \end{aligned} \tag{2.2}$$

The centroid ϵ that defines the location is given by $\epsilon = M_1$. Then the central moments $\mathcal{M}_r$ are given by

$$\begin{aligned} \mathcal{M}_r &= \int_{-\infty}^{+\infty} (x-\epsilon)^r \rho(x)dx \\ &= \sum_{p=0}^{r} \binom{r}{p} (-1)^{r-p} M_p \, \epsilon^{r-p} \end{aligned} \tag{2.3}$$

The second equality in the above equation gives the relationship between central and non-central moments. The width σ, of $\rho(x)$, that defines the scale is given by $\sigma = \mathcal{M}_2^{1/2}$ and the variance $\sigma^2 = \mathcal{M}_2$. Just as M_r's derive from $\phi(t)$, the cumulants K_r derive from $\ell n\, \phi(t)$ and they are related to the central moments $\mathcal{M}_r$; $\ell n\, \phi(t) = \sum_{r>0} \frac{(it)^r}{r!} K_r$. Similarly, the reduced central moments $\mu_r = \frac{\mathcal{M}_r}{\sigma^r}$,

$$\mu_r = \int_{-\infty}^{+\infty} \left(\frac{x-\epsilon}{\sigma}\right)^r \rho(x)dx \tag{2.4}$$

define the reduced cumulants $k_r = K_r/\sigma^r$. It is useful to point out that the cumulants K_r add under convolution. Before giving the relationship between K_r's and $\mathcal{M}_r$'s and other details, let us define the Gaussian density $\rho_{\mathcal{G}}(x)$ and the standard Gaussian $\eta_{\mathcal{G}}(\hat{x})$ which involves standardized variable $\hat{x}$,

$$\begin{aligned}
\rho_{\mathcal{G}}(x) &= \frac{1}{\sqrt{2\pi}\sigma} exp\left\{-\frac{(x-\epsilon)^2}{2\sigma^2}\right\}; \\
\eta_{\mathcal{G}}(\hat{x}) &= \frac{1}{\sqrt{2\pi}} exp\left\{-\frac{\hat{x}^2}{2}\right\} \\
\hat{x} &= (x - M_1)/(M_2 - M_1^2)^{1/2} = (x-\epsilon)/\sigma\,, \\
\rho_{\mathcal{G}}(x)dx &= \eta_{\mathcal{G}}(\hat{x})d\hat{x}.
\end{aligned} \tag{2.5}$$

One very important property is that all the cumulants K_r $(r > 2)$ are zero for a Gaussian. This follows from the results that $\mu_r = 0$ for r odd and $\mu_r = (r-1)!!$ for r even for a Gaussian density. Therefore $K_r (r > 2)$ are called shape parameters and in particular, $k_3 = \gamma_1$ is called skewness and $k_4 = \gamma_2$ is the excess. The relationships between the cumulants $(K_r,\, k_r)$ and the reduced central moments μ_r are (for $r \leq 6$),

$$\begin{aligned}
&K_1 = \epsilon, \quad K_2 = \sigma^2, \quad k_3 = \mu_3, \quad k_4 = \mu_4 - 3 \\
k_5 &= \mu_5 - 10\mu_3, \quad k_6 = \mu_6 - 15\mu_4 - 10\mu_3^2 + 30
\end{aligned} \tag{2.6}$$

In general, one can seek an expansion of a given distribution ρ in terms of the cumulants k_r, by starting with the Gaussian density ρ_G,

$$\begin{aligned} \rho(x)dx &= \eta(\hat{x})d\hat{x}, \\ \eta(\hat{x}) &= exp\left\{\sum_{r\geq 3}\frac{(-1)^r}{r!}k_r D_{\hat{x}}^r\right\}\eta_G(\hat{x}) \end{aligned} \tag{2.7}$$

The Edgeworth (Ed) expansion which is asymptotically convergent assumes that the cumulants $k_r \propto 1/p^{r-2}$ for $r \geq 3$ where p is a parameter of the system under consideration. Collecting terms upto order $1/p$ in (2.7) (thus incorporating γ_1, γ_2 corrections) gives the Edgeworth corrected Gaussian which is denoted by η_{Ed},

$$\eta_{Ed}(\hat{x}) = \eta_G(\hat{x})\left\{1 + \left[\frac{\gamma_1}{6}He_3(\hat{x})\right] + \left[\frac{\gamma_2}{24}He_4(\hat{x}) + \frac{\gamma_1^2}{72}He_6(\hat{x})\right]\right\} ,$$

$$\begin{aligned} &He_0(\hat{x}) = 1,\ He_1(\hat{x}) = \hat{x},\ He_2(\hat{x}) = \hat{x}^2 - 1, \\ &He_3(\hat{x}) = \hat{x}^3 - 3\hat{x},\ He_4(\hat{x}) = \hat{x}^4 - 6\hat{x}^2 + 3, \\ &He_5(\hat{x}) = \hat{x}^5 - 10\hat{x}^3 + 15\hat{x}, \\ &He_6(\hat{x}) = \hat{x}^6 - 15\hat{x}^4 + 45\hat{x}^2 - 15 \end{aligned} \tag{2.8}$$

In (2.8) $He_r(\hat{x})$ are Hermite polynomials. In applying (2.7) and (2.8) it should be kept in mind that the centroid and the width of $\rho(x)$ and $\rho_G(x)$ should be kept identical. Finally, it is useful to mention that corresponding to a given $\rho(x)$, one can define a set of orthonormal polynomials $P_\mu(x)$ such that $\int_{-\infty}^{+\infty} P_\mu(x)P_\nu(x)\rho(x)dx = \delta_{\mu\nu}$. Explicit form of the polynomials $P_\mu(x)$ in terms of the moments of $\rho(x)$ is

$$P_\mu(x) = [D_\mu D_{\mu-1}]^{-1/2}\begin{vmatrix} 1 & M_1 & - & - & - & M_\mu \\ M_1 & M_2 & - & - & - & M_{\mu+1} \\ - & - & - & - & - & - \\ - & - & - & - & - & - \\ M_{\mu-1} & M_\mu & - & - & - & M_{2\mu-1} \\ 1 & x & x^2 & - & - & x^\mu \end{vmatrix} ;$$

$$D_\mu = \begin{vmatrix} 1 & M_1 & - & - & - & M_\mu \\ M_1 & M_2 & - & - & - & M_{\mu+1} \\ - & - & - & - & - & - \\ - & - & - & - & - & - \\ M_\mu & M_{\mu+1} & - & - & - & M_{2\mu} \end{vmatrix} \tag{2.9}$$

For example $P_1(x)$ and $P_2(x)$ for a given density $\rho(x)$ are $P_1(x) = \hat{x}$, $P_2(x) = (\hat{x}^2 - \gamma_1\hat{x} - 1)/(\gamma_2 + 2 - \gamma_1^2)^{1/2}$. The Hermite polynomials $He_\mu(\hat{x}) = (-1)^\mu \eta_G^{-1}(\hat{x}) \frac{\partial^\mu}{\partial \hat{x}^\mu}\eta_G(\hat{x})$ are in fact orthogonal polynomials with respect to the standard Gaussian $\eta_G(\hat{x})$.

2.2.2 Bivariate distributions

Many of the properties of bivariate distributions are similar to that of univariate distributions and therefore much of the discussion in this subsection is in the same lines as in the previous subsection. Given a bivariate joint probability density (or simply a bivariate density) $\rho(x_1, x_2)$, at the outset it is assumed that it is positive definite and normalized to unity,

$$\int_{-\infty}^{+\infty}\int \rho(x_1, x_2)dx_1dx_2 = 1,$$

$$\rho(x_1, x_2) \geq 0\,;\ -\infty \leq x_1 \leq +\infty,\ -\infty \leq x_2 \leq +\infty\,. \tag{2.10}$$

The Fourier transform of $\rho(x_1, x_2)$ gives the bivariate characteristic function $\phi(t_1, t_2)$ whose expansion in powers of t_1 and t_2 defines the bivariate moments M_{rs} and a simple expression for M_{rs} is,

$$M_{rs} = \int_{-\infty}^{+\infty}\int x_1^r x_2^s \rho(x_1, x_2)dx_1dx_2. \tag{2.11}$$

The eigenvalue density $\rho_1(x_1)$ of x_1 is $\rho_1(x_1) = \int_{-\infty}^{+\infty} \rho(x_1, x_2)dx_2$ and in connection with $\rho(x_1, x_2)$, it is referred to as the marginal density (similarly $\rho_2(x_2)$ is defined). The centroids $\epsilon_1(\epsilon_2)$ of the marginal densities $\rho_1(\rho_2)$ are related to the moments M_{rs} by the relations $\epsilon_1 = M_{10}$ and $\epsilon_2 = M_{01}$. The bivariate central moments $\mathcal{M}_{rs}$ are given by,

$$\mathcal{M}_{rs} = \int_{-\infty}^{+\infty}\int (x_1 - M_{10})^r (x_2 - M_{01})^s \rho(x_1, x_2)dx_1 dx_2 \qquad (2.12)$$

and it is easy to write $\mathcal{M}_{rs}$ in terms of the non-central moments M_{rs}. The $\sigma_1 = \mathcal{M}_{20}^{1/2}$ and $\sigma_2 = \mathcal{M}_{02}^{1/2}$ are the widths of the marginal densities $\rho_1(x_1)$ and $\rho_2(x_2)$ respectively. The central moments $\mathcal{M}_{rs}$ define the bivariate cumulants K_{rs}; K_{rs} derive from $\ell n\, \phi(t_1, t_2)$ just as M_{rs} derive from $\phi(t_1, t_2)$. Similarly the bivariate reduced central moments $\mu_{rs} = \mathcal{M}_{rs}/\sigma_1^r \sigma_2^s$,

$$\mu_{rs} = \int_{-\infty}^{+\infty}\int \left(\frac{x_1 - M_{10}}{\sigma_1}\right)^r \left(\frac{x_2 - M_{01}}{\sigma_2}\right)^s \rho(x_1, x_2)dx_1 dx_2\,, \qquad (2.13)$$

define the reduced cumulants $k_{rs} = K_{rs}/\sigma_1^r \sigma_2^s$. The k_{11} cumulant defines the bivariate correlation coefficient ζ,

$$\zeta = k_{11} = \mu_{11} = \int_{-\infty}^{+\infty}\int \left(\frac{x_1 - \epsilon_1}{\sigma_1}\right)\left(\frac{x_2 - \epsilon_2}{\sigma_2}\right) \rho(x_1, x_2)dx_1 dx_2\,. \qquad (2.14)$$

Before going further let us first introduce the bivariate Gaussian density $\rho_{BIV-\mathcal{G}}$ which is defined in terms of the five variables (ϵ_1, ϵ_2, σ_1, σ_2, ζ),

$$\rho_{BIV-\mathcal{G}}(x_1, x_2) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\zeta^2}} \times$$

$$exp\left\{ -\frac{\left[\left(\frac{x_1 - \epsilon_1}{\sigma_1}\right)^2 - 2\zeta\left(\frac{x_1 - \epsilon_1}{\sigma_1}\right)\left(\frac{x_2 - \epsilon_2}{\sigma_2}\right) + \left(\frac{x_2 - \epsilon_2}{\sigma_2}\right)^2\right]}{2(1-\zeta^2)} \right\} \qquad (2.15)$$

One very important property is that k_{rs} for $r+s \geq 3$ are all zero for a bivariate Gaussian. In Chapters 3 - 6 the suffix BIV is dropped whenever there is no confusion. The standard bivariate Gaussian $\eta_{\mathcal{G}}(\hat{x}_1, \hat{x}_2)$ and the relationship between $\eta_{\mathcal{G}}$ and $\rho_{\mathcal{G}}$, involving the standardized variables $(\hat{x}_1, \hat{x}_2)$; $\hat{x}_1 = (x_1 - \epsilon_1)/\sigma_1$, $\hat{x}_2 = (x_2 - \epsilon_2)/\sigma_2$, are

$$\begin{aligned} \rho_{\mathcal{G}}(x_1, x_2)dx_1dx_2 &= \eta_{\mathcal{G}}(\hat{x}_1, \hat{x}_2)d\hat{x}_1d\hat{x}_2\,, \\ \eta_{\mathcal{G}}(\hat{x}_1, \hat{x}_2) &= \frac{1}{2\pi\sqrt{(1-\zeta^2)}} exp\left\{-\frac{\hat{x}_1^2 - 2\zeta\hat{x}_1\hat{x}_2 + \hat{x}_2^2}{2(1-\zeta^2)}\right\} \end{aligned} \tag{2.16}$$

Following (2.16), $\rho(x_1, x_2)$ is expressible in terms of $\eta(\hat{x}_1, \hat{x}_2)$ where,

$$\eta(\hat{x}_1, \hat{x}_2)d\hat{x}_1d\hat{x}_2 = \rho(x_1, x_2)dx_1dx_2 \tag{2.17}$$

For a general bivariate density $\rho(x_1, x_2)$ the higher order cumulants (shape parameters) k_{rs} for $r+s \geq 3$ are non-zero and it is easy to write down k_{rs} in terms of μ_{rs} (or $\mathcal{M}_{rs}$). The relationships for $r+s \leq 4$ are (see [Ke-69] for more details),

$$\begin{gathered} K_{10} = M_{10} = \epsilon_1, \quad K_{01} = M_{01} = \epsilon_2, \\ K_{20} = \mathcal{M}_{20} = \sigma_1 \quad K_{02} = \mathcal{M}_{02} = \sigma_2 \\ k_{11} = \mu_{11} = \zeta \\ k_{30} = \mu_{30}, \quad k_{21} = \mu_{21}, \quad k_{12} = \mu_{12}, \quad k_{03} = \mu_{03} \\ k_{40} = \mu_{40} - 3, \quad k_{31} = \mu_{31} - 3\zeta, \quad k_{22} = \mu_{22} - 1 - 2\zeta^2 \\ k_{13} = \mu_{13} - 3\zeta, \quad k_{04} = \mu_{04} - 3 \end{gathered} \tag{2.18}$$

Once again it should be pointed out that the bivariate cumulants K_{rs} add under bivariate convolution. Starting from a bivariate Gaussian density $\rho_{\mathcal{G}}$, one can seek an expansion of a general distribution ρ in terms of the cumulants k_{rs} using (2.18) and

$$\eta(\hat{x}_1, \hat{x}_2) = exp\left\{\sum_{r+s\geq 3} \frac{(-1)^{r+s}}{r!s!} k_{rs} D^r_{\hat{x}_1} D^s_{\hat{x}_2}\right\} \eta_{\mathcal{G}}(\hat{x}_1, \hat{x}_2) \tag{2.19}$$

The bivariate Ed expansion, which is asymptotically convergent, starts with the assumption that the cumulants $k_{rs} \propto 1/p^{r+s-2}$ for $r+s \geq 3$ where p is a parameter of the system described by $\rho(x_1, x_2)$, i.e. the existence of p is assumed. Expanding the exponential in (2.19) and collecting terms to orders $p^{-1/2}$, p^{-1}, $p^{-3/2}$, p^{-2} etc. give the Ed expansion in powers of $p^{-1/2}$. Using the bivariate Hermite polynomials $He_{m_1 m_2}(\hat{x}_1, \hat{x}_2)$,

$$He_{m_1 m_2}(\hat{x}_1, \hat{x}_2)\eta_G(\hat{x}_1, \hat{x}_2) = (-1)^{m_1+m_2} \frac{\partial}{\partial \hat{x}_1^{m_1}} \frac{\partial}{\partial \hat{x}_2^{m_2}} \eta_G(\hat{x}_1, \hat{x}_2), \tag{2.20}$$

the Ed expansion to order $1/p$ (here one needs k_{rs} with $r+s \leq 4$) is explicitly given by (hereafter denoted as η_{BIV-Ed} or ρ_{BIV-Ed}),

$$\begin{aligned}
\eta_{BIV-Ed}(\hat{x}_1, \hat{x}_2) &= \left\{1 + \left(\frac{k_{30}}{6} He_{30}(\hat{x}_1, \hat{x}_2) + \frac{k_{21}}{2} He_{21}(\hat{x}_1, \hat{x}_2)\right.\right. \\
&+ \left.\frac{k_{12}}{2} He_{12}(\hat{x}_1, \hat{x}_2) + \frac{k_{03}}{6} He_{03}(\hat{x}_1, \hat{x}_2)\right) \\
&+ \left(\left\{\frac{k_{40}}{24} He_{40}(\hat{x}_1, \hat{x}_2) + \frac{k_{31}}{6} He_{31}(\hat{x}_1, \hat{x}_2)\right.\right. \\
&+ \left.\left.\frac{k_{22}}{4} He_{22}(\hat{x}_1, \hat{x}_2) + \frac{k_{13}}{6} He_{13}(\hat{x}_1, \hat{x}_2) + \frac{k_{04}}{24} He_{04}(\hat{x}_1, \hat{x}_2)\right\}\right. \\
&+ \left\{\frac{k_{30}^2}{72} He_{60}(\hat{x}_1, \hat{x}_2) + \frac{k_{30}k_{21}}{12} He_{51}(\hat{x}_1, \hat{x}_2)\right. \\
&+ \left[\frac{k_{21}^2}{8} + \frac{k_{30}k_{12}}{12}\right] He_{42}(\hat{x}_1, \hat{x}_2) \\
&+ \left[\frac{k_{30}k_{03}}{36} + \frac{k_{12}k_{21}}{4}\right] He_{33}(\hat{x}_1, \hat{x}_2) \\
&+ \left[\frac{k_{12}^2}{8} + \frac{k_{21}k_{03}}{12}\right] He_{24}(\hat{x}_1, \hat{x}_2) + \frac{k_{12}k_{03}}{12} He_{15}(\hat{x}_1, \hat{x}_2) \\
&+ \left.\left.\left.\frac{k_{03}^2}{72} He_{06}(\hat{x}_1, \hat{x}_2)\right\}\right)\right\} \eta_G(\hat{x}_1, \hat{x}_2)
\end{aligned} \tag{2.21}$$

The expression (2.21) together with (2.16, 2.17) is referred to in the text as Edgeworth corrected bivatiate Gaussian η_{BIV-Ed} or ρ_{BIV-Ed}. Finally the

Hermite polynomials $He_{m_1,m_2}(\hat{x}_1,\hat{x}_2)$ are calculated easily using the following relations,

$$
\begin{aligned}
&(1-\zeta^2)He_{m_1+1,m_2}(\hat{x}_1,\hat{x}_2) = (\hat{x}_1-\zeta\hat{x}_2)He_{m_1,m_2}(\hat{x}_1,\hat{x}_2) \\
&\quad -m_1He_{m_1-1,m_2}(\hat{x}_1,\hat{x}_2)+m_2\zeta He_{m_1,m_2-1}(\hat{x}_1,\hat{x}_2);
\end{aligned}
$$

$$
\begin{aligned}
He_{00}(\hat{x}_1,\hat{x}_2) &= 1 \\
He_{10}(\hat{x}_1,\hat{x}_2) &= \frac{\hat{x}_1-\zeta\hat{x}_2}{1-\zeta^2} \\
He_{01}(\hat{x}_1,\hat{x}_2) &= \frac{\hat{x}_2-\zeta\hat{x}_1}{1-\zeta^2} \\
He_{11}(\hat{x}_1,\hat{x}_2) &= \frac{(\hat{x}_1-\zeta\hat{x}_2)(\hat{x}_2-\zeta\hat{x}_1)}{(1-\zeta^2)^2}+\frac{\zeta}{1-\zeta^2}
\end{aligned}
\tag{2.22}
$$

The probability densities $\rho_{12}(x_1|x_2)$ and $\rho_{21}(x_2|x_1)$ that are referred to as the conditional densities are given by,

$$
\begin{aligned}
\rho_{12}(x_1|x_2) &= \rho(x_1,x_2)/\rho_2(x_2) \\
\rho_{21}(x_2|x_1) &= \rho(x_1,x_2)/\rho_1(x_1).
\end{aligned}
\tag{2.23}
$$

The conditional moments $M_p(x_2)$ of ρ_{12} (and similarly $M_p(x_1)$ of ρ_{21}) are

$$
\begin{aligned}
M_p(x_2) &= \int_{-\infty}^{+\infty} x_1^p\rho_{12}(x_1|x_2)dx_1 \\
&= \int_{-\infty}^{+\infty} x_1^p\rho(x_1,x_2)dx_1 \Big/ \int_{-\infty}^{+\infty}\rho(x_1,x_2)dx_1.
\end{aligned}
\tag{2.24}
$$

It is important to note that given $\eta_{BIV-\mathcal{G}}$, the corresponding conditional densities will be Gaussians,

$$
\eta_{12;\mathcal{G}}(\hat{x}_1|\hat{x}_2) = \frac{1}{\sqrt{2\pi(1-\zeta^2)}}exp\left\{-\frac{(\hat{x}_1-\zeta\hat{x}_2)^2}{2(1-\zeta^2)}\right\}. \tag{2.25}
$$

Therefore, for a bivariate Gaussian, conditional centroids are linear in the fixed variable with the slope given by correlation coefficient. Similarly the conditional width is a constant and it is a simple function of the bivariate correlation coefficient.

2.3 State, expectation value and strength densities: CLT results

2.3.1 State densities

Given a hamiltonian H acting in a m-particle space, the state density $I^m(E)$ and the corresponding normalized density $\rho^m(E)$ are defined by

$$\begin{aligned} I^m(E) &= \sum_r g_r \delta(E - E_r) = \langle\langle \delta(H - E) \rangle\rangle^m \\ &= \sum_{\alpha \in m} \langle m\alpha | \delta(H - E) | m\alpha \rangle = d(m) \langle \delta(H - E) \rangle^m \\ &= d(m) \rho^m(E) \end{aligned} \tag{2.26}$$

In the above equation g_r is the degeneracy of r^{th} eigenvalue E_r, $d(m)$ is m-particle space dimensionality, $\langle\langle\ \rangle\rangle^m$ denotes m-particle trace and $\langle\ \rangle^m$ is m-particle average. Using the definition of $\rho^m(E)$ in (2.26), the moments M_r (2.2) and the corresponding central moments $\mathcal{M}_r$ (2.3) for $\rho^m(E)$ are

$$M_r(m) = \langle H^r \rangle^m; \quad \mathcal{M}_r(m) = \langle (H - \langle H \rangle^m)^r \rangle^m \tag{2.27}$$

As stated in Chapter 1, due to CLT action in strongly interacting m-particle spaces, $\rho^m(E)$ takes a Gaussian form defined by the centroid $\epsilon_H(m) = \epsilon(m) = \langle H \rangle^m$ and variance $\sigma_H^2(m) = \sigma^2(m) = \langle (H - \epsilon(m))^2 \rangle^m$,

$$\rho^m(E) \overset{CLT}{\longrightarrow} \rho_G^m(E) = \frac{1}{\sqrt{2\pi}\sigma} exp\left\{ -\frac{(E - \epsilon(m))^2}{2\sigma^2(m)} \right\} \tag{2.28}$$

By using Edgeworth corrected Gaussian given by (2.8), the departures from CLT result as represented by non-zero skewness γ_1 and excess γ_2 values can be taken into account. From now onwards the suffix m appearing in (2.26 - 2.28) is dropped when there is no confusion.

2.3.2 Expectation values and expectation value densities

Formally the expectation value $\langle K\rangle^E$ of an operator K is defined by

$$\langle K\rangle^E = \left[\sum_{\alpha\in E}\langle E\alpha|K|E\alpha\rangle\right] \Big/ I(E) = I_K(E)/I(E) \tag{2.29}$$

where the expectation value denstity $I_K(E)$ is,

$$I_K(E) = \langle K\rangle^E I(E) = \langle\langle K\delta(H-E)\rangle\rangle^m. \tag{2.30}$$

Definition of $\langle K\rangle^E$ as given by (2.29) takes into account properly the degeneracies in the spectrum and because of this one is led to consider expectation value densities. Observables like spherical-orbit occupancies, spin-cutoff factors, static moments etc. are expressible as expectation values. Using the property $\delta(H-E) = \rho(E)\sum_\mu P_\mu(H)P_\mu(E)$, of the orthogonal polynomials $P_\mu(E)$ defined by (2.9) with respect to $\rho(E)$, an expansion of $\langle K\rangle^E$ in terms of traces can be written down

$$\langle K\rangle^E = \sum_{\mu=0}^{\infty}\langle KP_\mu(H)\rangle^m P_\mu(E) \underset{\mu=0,1}{\overset{CLT}{\longrightarrow}} \epsilon_K(m) + \langle\hat{K}\hat{H}\rangle^m\sigma_K(m)\hat{E} \tag{2.31}$$

In (2.31) $\hat{K}$ and $\hat{H}$ are standard operators and following (2.5), $\hat{K} = (K - \epsilon_K(m))/\sigma_K(m)$ and $\hat{H} = (H-\epsilon_H(m))/\sigma_H(m)$. Similarly $\hat{E} = (E-\epsilon_H(m))/\sigma_H(m)$. Note that $\langle\hat{K}\hat{H}\rangle$ is nothing but the correlation coefficient ζ_{K-H}. The CLT result which shows linear behavior of $\langle K\rangle^E$ with respect to E (see Fig. 1.3a

for an example) follows immediately by considering the deformation $H \rightarrow H + \alpha K \Longrightarrow \rho \rightarrow \rho_\alpha$ and assuming that CLT applies for ρ as well as ρ_α densities. An alternative to the polynomial expansion method (2.31) which is more appropriate for the operators of the form $\mathcal{O}^\dagger\mathcal{O}$ is to directly construct the expectation value densities $I_K(E)$ defined in (2.30) in terms of its moments. With $K = \mathcal{O}^\dagger\mathcal{O}$ being positive definite operator, $I_K(E)$ can be treated as a probability distribution function and this gives the following important result,

$$\langle K\rangle^E = I_K(E)/I(E) \overset{CLT}{\longrightarrow} I_{K:\mathcal{G}}(E)/I_{\mathcal{G}}(E) \tag{2.32}$$

The origin of the CLT result given in (2.32) lies in the bivariate Gaussian form for strength densities given by (2.39) ahead. The normalized density $\rho_K(E)$ and the corresponding moments $M_r(K)$ are defined by

$$\begin{aligned} \rho_K(E) &= I_K(E)/\langle\langle K\rangle\rangle \\ \widetilde{M}_r(K) &= \langle KH^r\rangle \\ M_r(K) &= \widetilde{M}_r(K)/\widetilde{M}_0(K) = \langle KH^r\rangle/\langle K\rangle \end{aligned} \tag{2.33}$$

The moments $\widetilde{M}_r(K)$, defined in (2.33), of $I_K(E)$ can be derived by parametric differentiation of the moments $M_r(\alpha)$ of ρ_α produced by $H_\alpha = H + \alpha K$,

$$\widetilde{M}_r(K) = (r+1)^{-1} \lim_{\alpha\rightarrow 0} \frac{\partial}{\partial\alpha}[M_{r+1}(\alpha)] \tag{2.34}$$

For an operator of the type $K = T^2$ with the commutator $[T, H] = 0$, one can write $\langle KH^r\rangle = \langle T^2H^r\rangle$ traces, by double parametric differentiation, in terms of the moments of ρ_α produced by $H \rightarrow H + \alpha T$,

$$\langle T^2H^r\rangle = [(r+1)(r+2)]^{-1} \lim_{\alpha\rightarrow 0} \frac{\partial^2}{\partial\alpha^2}[\langle H + \alpha T\rangle^{r+2}] \tag{2.35}$$

Results given by (2.26) - (2.35) are used in Chapter 3.

2.3.3 Strength densities

The strength $R_{\mathcal{O}}(E, E')$ for a transition operator $\mathcal{O}$, is the square of the matrix element connecting the eigenstates with energies E and E' (assuming no degeneracies for the eigenvalues E and E')

$$R_{\mathcal{O}}(E, E') = |\langle E'm'|\mathcal{O}|Em\rangle|^2 \tag{2.36}$$

The corresponding strength density $\mathbf{I}_{\mathcal{O}}(E, E')$, which properly takes care of degeneracies, is defined by,

$$\begin{aligned}
\mathbf{I}_{\mathcal{O}}^{H;m,m'}(E, E') &= I^{m'}(E')\,|\langle E'm'|\mathcal{O}|Em\rangle|^2\, I^{m}(E) \\
&= \langle\langle \mathcal{O}^\dagger \delta(H - E')\mathcal{O}\delta(H - E)\rangle\rangle^m \ ; \\
\rho_{\mathcal{O};BIV}^{H;m,m'} &= \langle \mathcal{O}^\dagger \delta(H - E')\mathcal{O}\delta(H - E)\rangle^m / \langle \mathcal{O}^\dagger \mathcal{O}\rangle^m
\end{aligned} \tag{2.37}$$

In (2.37) ρ is normalized bivariate strength density (for non-zero $\langle \mathcal{O}^\dagger \mathcal{O}\rangle$). As $\mathbf{I}_{\mathcal{O}}(E, E')$ is positive definite, it can be represented by a bivariate probability distribution function and therefore the results of Sect. 2.2.2 will apply. The trace expressions for the centroids and variances of the marginal densities $I_1(E)$ and $I_2(E')$, the bivariate correlation coefficient ζ and for the reduced central moments μ_{pq} are given below:

$$\begin{aligned}
\epsilon_1 &= \langle \mathcal{O}^\dagger \mathcal{O} H\rangle^m / \langle \mathcal{O}^\dagger \mathcal{O}\rangle^m \\
\epsilon_2 &= \langle \mathcal{O}^\dagger H \mathcal{O}\rangle^m / \langle \mathcal{O}^\dagger \mathcal{O}\rangle^m \\
\sigma_1^2 &= \langle \mathcal{O}^\dagger \mathcal{O} H^2\rangle^m / \langle \mathcal{O}^\dagger \mathcal{O}\rangle^m - \epsilon_1^2 \\
\sigma_2^2 &= \langle \mathcal{O}^\dagger H^2 \mathcal{O}\rangle^m / \langle \mathcal{O}^\dagger \mathcal{O}\rangle^m - \epsilon_2^2 \\
\zeta &= \left\langle \mathcal{O}^\dagger \left(\frac{H - \epsilon_2}{\sigma_2}\right) \mathcal{O} \left(\frac{H - \epsilon_1}{\sigma_1}\right) \right\rangle^m \Big/ \langle \mathcal{O}^\dagger \mathcal{O}\rangle^m \\
\mu_{pq} &= \left\langle \mathcal{O}^\dagger \left(\frac{H - \epsilon_2}{\sigma_2}\right)^q \mathcal{O} \left(\frac{H - \epsilon_1}{\sigma_1}\right)^p \right\rangle^m \Big/ \langle \mathcal{O}^\dagger \mathcal{O}\rangle^m
\end{aligned} \tag{2.38}$$

The CLT result (smoothed form) for $\mathbf{I}_{\mathcal{O}}(E,E')$ under some plausible arguments is that $\rho(E,E')$ takes a bivariate Gaussian form

$$\rho(E,E') \overset{CLT}{\longrightarrow} \rho_{BIV-\mathcal{G}}(E,E') \tag{2.39}$$

Explicit form of $\rho_{BIV-\mathcal{G}}(E,E')$ is given by (2.15). It has very important consequences for non-energy weighted sum rule or sum strength (NEWSR), for the strength centroid, strength width etc. The strength moments $M_{\mathsf{P}}(E)$ originating from energy E are defined by (assuming that the states $|E\rangle$ and $|E'\rangle$ are non- degenerate)

$$M_P(E) = \sum_{E'} (E')^P |\langle E'|\mathcal{O}|E\rangle|^2 \tag{2.40}$$

In continuous version (2.40) becomes

$$\begin{aligned} M_P(E) &= [I(E)]^{-1} \int \mathbf{I}_{\mathcal{O}}(E,E')(E')^P dE' \\ &= \frac{I_{1;\mathcal{O}}(E)}{I(E)} \int \rho_{21;\mathcal{O}}(E'|E)(E')^P dE' \end{aligned} \tag{2.41}$$

In (2.41), $I(E)$ is state density, $I_{1;\mathcal{O}}(E) = \langle\langle \mathcal{O}^\dagger \mathcal{O} \delta(H-E)\rangle\rangle = \langle\langle \mathcal{O}^\dagger \mathcal{O}\rangle\rangle \rho_{1;\mathcal{O}}(E)$ is one of the marginal densities (similarly $I_{2;\mathcal{O}}(E')$ is defined) corresponding to $\mathbf{I}_{\mathcal{O}}(E,E')$ and $\rho_{21;\mathcal{O}}(E'|E)$ is one of the conditional densities corresponding to $\rho_{\mathcal{O};BIV}(E,E')$; Sect. 2.2.2 gives definitions and properties for marginal and conditional densities. With $(\epsilon_c\ ,\ \sigma_c)$, $(\epsilon_1\ ,\ \sigma_1)$ and $(\epsilon_2\ ,\ \sigma_2)$, the centroid and width of $I(E)$, $I_{1;\mathcal{O}}(E)$ and $I_{2;\mathcal{O}}(E')$ the bivariate Gaussian form of $\mathbf{I}_{\mathcal{O}}(E,E')$ and the Gaussian form of $I(E)$ give simple expressions for NEWSR which equals to $M_0(E)$, the strength centroid $\epsilon(E) = M_1(E)/M_0(E)$ and strength width $\sigma(E) = \{M_2(E)/M_0(E) - [M_1(E)/M_0(E)]^2\}^{1/2}$ (follow easily from (2.15, 2.25, 2.5)),

$$
\begin{aligned}
M_0(E) &\overset{CLT}{\longrightarrow} \langle \mathcal{O}^\dagger \mathcal{O} \rangle \frac{\sigma_c}{\sigma_1} exp\left\{ -\frac{1}{2}\left[\left(\frac{E-\epsilon_1}{\sigma_1} \right)^2 - \left(\frac{E-\epsilon_c}{\sigma_c} \right)^2 \right] \right\}, \\
\epsilon(E) &\overset{CLT}{\longrightarrow} \epsilon_2 + \zeta \frac{\sigma_2}{\sigma_1}(E-\epsilon_1) \\
\sigma(E) &\overset{CLT}{\longrightarrow} \sigma_2(1-\zeta^2)^{1/2}. \qquad (2.42)
\end{aligned}
$$

Results given by (2.42) are well verified in Fig. 1.4 and they are used in Chapter 6.

2.4 Partitioning : spherical and unitary configurations

As stated in Chapter 1, in order to extend the applicability of CLT results given in Sect. 2.3 to large spaces, to improve the accuracy of the predictions based on CLT results (including Edgeworth corrections) and to bring in more information it is essential to partition the m-particle spaces to subspaces. Simple partitioning of m-particle spaces is according to spherical and unitary configurations and in order to define them, we begin with m-particles distributed over spherical shell model j-orbits (single particle s.p. orbits) denoted by α, β etc. (j_α being the angular momentum and $N_\alpha = 2j_\alpha + 1$ is the degeneracy of the orbit α). The m-particle spectroscopic space can be decomposed into spherical configurations $\mathbf{m} = (m_\alpha, m_\beta ...)$ where m_α is the number of particles in the orbit α and $m = \sum_\alpha m_\alpha ; m = \sum \mathbf{m}$. Note that the dimensionality $d(\mathbf{m})$ of the configuration $\mathbf{m}$ is $d(\mathbf{m}) = \prod_\alpha \begin{pmatrix} N_\alpha \\ m_\alpha \end{pmatrix}$. For example, for identical particles, denoting $1d_{5/2}$, $2s_{1/2}$ and $1d_{3/2}$ orbits as #1, #2 and #3 orbits,

$(ds)^4$ spherical configurations are $\mathbf{m} = (m_1, m_2, m_3) = (4,0,0) \oplus (3,1,0) \oplus (3,0,1) \oplus (2,2,0) \oplus (2,1,1) \oplus (2,0,2) \oplus (1,2,1) \oplus (1,1,2) \oplus (1,0,3) \oplus (0,2,2) \oplus (0,1,3) \oplus (0,0,4)$. A unitary orbit $\boldsymbol{\alpha}$ is defined as a set of spherical orbits. With this, decomposition of m-particle space into unitary configurations [m] is possible; $m \rightarrow \sum[\mathbf{m}]$. As above, a unitary configuration $[\mathbf{m}] = (m_{\boldsymbol{\alpha}}, m_{\boldsymbol{\beta}}, ...)$; $m = \sum m_{\boldsymbol{\alpha}}$. Using the convention that the spherical orbits α belong to unitary orbit $\boldsymbol{\alpha}$ and similarly the orbits β belong to $\boldsymbol{\beta}$ etc., the number of s.p. states in a unitary orbit $\boldsymbol{\alpha}$ is $N_{\boldsymbol{\alpha}} = \sum_{\alpha \in \boldsymbol{\alpha}} N_\alpha$. The dimensionality of the configuration [m] is $d([\mathbf{m}]) = \prod_{\boldsymbol{\alpha}} \begin{pmatrix} N_{\boldsymbol{\alpha}} \\ m_{\boldsymbol{\alpha}} \end{pmatrix}$. For example in the above ds-shell case one can choose $(1d_{5/2}, 2s_{1/2})$ and $(1d_{3/2})$ to be two unitary orbits (#1, #2 orbits) and then $(ds)^4 \rightarrow [\mathbf{m}] = (m_1, m_2) = (4,0) \oplus (3,1) \oplus (2,2) \oplus (1,3) \oplus (0,4)$. It is important to recognize that $[\mathbf{m}] \rightarrow \sum \mathbf{m}$ and the set of spherical configurations $\mathbf{m}$ that belong to a given unitary configuration is easy to enumerate. For example in the above case, $(4,0) \rightarrow (4,0,0) \oplus (3,1,0) \oplus (2,2,0)$; $(3,1) \rightarrow (3,0,1) \oplus (2,1,1) \oplus (1,2,1)$ etc. With spherical or unitary configurations, the decomposition of m-particle space is,

$$m \rightarrow \sum[\mathbf{m}]\,; \; [\mathbf{m}] \rightarrow \sum \mathbf{m}. \tag{2.43}$$

It is worth remarking that the decomposition given by (2.43) automatically produces fixed-parity subspaces by choosing the unitary orbits $\boldsymbol{\alpha}$ to be set of spherical orbits with all of them having same parity. One remarkable result is that under the above partitioning of the shell model space the state density $I^m(E)$ decomposes exactly into sum of partial $I^{\mathbf{m}}(E)$ and $I^{[\mathbf{m}]}(E)$ densities,

$$\begin{aligned} I^{H,m}(E) = \sum_{[\mathbf{m}]} I^{H,[\mathbf{m}]}(E) = \sum_{[\mathbf{m}]} \left\{ \sum_{\mathbf{m} \in [\mathbf{m}]} I^{H,\mathbf{m}}(E) \right\}\,; \\ I^{H,[\mathbf{m}]}(E) = \langle\langle \delta(H-E) \rangle\rangle^{[\mathbf{m}]}\,, \\ I^{H,\mathbf{m}}(E) = \langle\langle \delta(H-E) \rangle\rangle^{\mathbf{m}} \end{aligned} \tag{2.44}$$

It is important to recognize that corresponding to m, m and $[\mathrm{m}]$ there are group structures associated with them as given in Sect. 2.5 ahead. The moments $M_p(\mathrm{m})$ of $I^{H,\mathrm{m}}(E)$ and $M_p([\mathrm{m}])$ of $I^{H,[\mathrm{m}]}(E)$ are easily defined as traces of H^p over the corresponding subspaces,

$$\begin{aligned} M_p(\mathrm{m}) &= \langle H^p \rangle^{\mathrm{m}} \\ M_p([\mathrm{m}]) &= \langle H^p \rangle^{[\mathrm{m}]} = [d([\mathrm{m}])]^{-1} \sum_{\mathrm{m} \in [\mathrm{m}]} \langle\langle H^p \rangle\rangle^{\mathrm{m}} \\ &= \sum_{\mathrm{m} \in [\mathrm{m}]} \frac{d(\mathrm{m})}{d([\mathrm{m}])} M_p(\mathrm{m}) \end{aligned} \tag{2.45}$$

It should be recognized that unlike the scalar moments, $M_r(m)$ defined in (2.27), the fixed-m (similarly $[\mathrm{m}]$) moments involve intermediate configurations as the hamiltonian does not preserve these symmetries. For example the second moment $M_2(\mathrm{m})$ decomposes into partial moments $M_2(\mathrm{m} \to \mathrm{m}')$,

$$\begin{aligned} M_2(\mathrm{m}) &= [d(\mathrm{m})]^{-1} \langle\langle H^2 \rangle\rangle^{\mathrm{m}} \\ &= [d(\mathrm{m})]^{-1} \sum_{\mathrm{m}'} \sum_{\substack{\alpha \in \mathrm{m} \\ \beta \in \mathrm{m}'}} |\langle \mathrm{m}\alpha | H | \mathrm{m}'\beta \rangle|^2 \\ &= \sum_{\mathrm{m}'} M_2(\mathrm{m} \to \mathrm{m}'); \\ M_2(\mathrm{m} \to \mathrm{m}') &= [d(\mathrm{m})]^{-1} \sum_{\substack{\alpha \in \mathrm{m} \\ \beta \in \mathrm{m}'}} |\langle \mathrm{m}\alpha | H | \mathrm{m}'\beta \rangle|^2 \end{aligned} \tag{2.46}$$

With the centroids denoted by $\epsilon(\mathrm{m})$ and the variances denoted by $\sigma^2(\mathrm{m})$, the decomposition of $\sigma^2(\mathrm{m})$ into partial variances $\sigma^2(\mathrm{m} \to \mathrm{m}')$ ($\sigma^2(\mathrm{m} \to \mathrm{m})$ is called internal variance and $\sigma^2(\mathrm{m} \to \mathrm{m}')$; $\mathrm{m} \neq \mathrm{m}'$ is called external variance) is given by,

$$
\begin{aligned}
\sigma^2(\mathrm{m}) &= \sum_{\mathrm{m}'} \sigma^2(\mathrm{m} \rightarrow \mathrm{m}') \,, \\
\sigma^2(\mathrm{m} \rightarrow \mathrm{m}) &= M_2(\mathrm{m} \rightarrow \mathrm{m}) - (\epsilon(\mathrm{m}))^2 \,, \\
\sigma^2(\mathrm{m} \rightarrow \mathrm{m}') &= M_2(\mathrm{m} \rightarrow \mathrm{m}') \qquad (2.47)
\end{aligned}
$$

Just as the state densities decompose into partial densities, the expectation value densities also decompose into partial densities exactly in the same way. On the other hand decomposition of strength densities into partial densities still remains an unsolved problem. However there are ways to circumvent this problem; see Chapter 6.

Partitioning of the shell model space can be carried out in many different ways and the partitioning defined by irreducible representations (irreps) of groups that can be realized in shell model spaces (for example Wigner $SU(4)$, Elliot $SU(3)$, pairing $Sp(n)$ etc.) are in fact the most significant ones. The significance derives from the fact (as will be seen in Sects. 2.5 - 2.6) that the moments defined over the irreps in fact propagate from the few particle spaces to the many particle spaces and this is elaborated in Sect. 2.6. As mentioned earlier there are group structures associated with spherical and unitary configurations and before turning to this, it is useful to introduce the following symbols.

With m particles in N s.p. states, the number of holes $m^{\times} = N - m$. Similarly for m_α particles in N_α states, $m_\alpha^{\times} = N_\alpha - m_\alpha$ (note that $n_\alpha^{\times} = N_\alpha - n_\alpha$) and for $m_{\boldsymbol{\alpha}}$ particles in $N_{\boldsymbol{\alpha}}$ states, $m_{\boldsymbol{\alpha}}^{\times} = N_{\boldsymbol{\alpha}} - m_{\boldsymbol{\alpha}}$ (note that $n_{\boldsymbol{\alpha}}^{\times} = N_{\boldsymbol{\alpha}} - n_{\boldsymbol{\alpha}}$); spherical orbits and unitary orbits, spherical configurations and unitary configurations are already defined. Finally, the symbols $[X]_r$,

$X_{\alpha\beta....}$, $X_{\boldsymbol{\alpha\beta}.....}$, $\check{X}_{\alpha\beta}$ and $\check{X}_{\boldsymbol{\alpha\beta}}$ are defined as

$$\begin{aligned}
[X]_r &= X(X-1)(X-2).....(X-r+1); \\
X_{\alpha\beta\gamma...} &= X_\alpha(X_\beta - \delta_{\beta\alpha})(X_\gamma - \delta_{\gamma\alpha} - \delta_{\gamma\beta}).....; \\
X_{\boldsymbol{\alpha\beta\gamma}...} &= X_{\boldsymbol{\alpha}}(X_{\boldsymbol{\beta}} - \delta_{\boldsymbol{\beta\alpha}})(X_{\boldsymbol{\gamma}} - \delta_{\boldsymbol{\gamma\alpha}} - \delta_{\boldsymbol{\gamma\beta}}).....; \\
\check{X}_{\alpha\beta} &= X_\alpha(X_\beta - \delta_{\alpha\beta})/(1+\delta_{\alpha\beta}) \\
\check{X}_{\boldsymbol{\alpha\beta}} &= X_{\boldsymbol{\alpha}}(X_{\boldsymbol{\beta}} - \delta_{\boldsymbol{\alpha\beta}})/(1+\delta_{\boldsymbol{\alpha\beta}}) \\
& \qquad X = m,\ N,\ m^{\times},\ n,\ n^{\times} \qquad (2.48)
\end{aligned}$$

2.5 Unitary decomposition of operators

2.5.1 $U(N)$ group

With m identical fermions distributed over N single particle states, one can recognize the appearence of $U(N)$ group which is generated by the N^2 operators $a^\dagger_{j_\alpha m_\alpha} a_{j_\beta m_\beta}$; $\alpha, \beta = 1,2,...,N$. Then the $\begin{pmatrix} N \\ m \end{pmatrix}$ antisymmetric states form an irrep of the group $U(N)$, usually denoted by Young shape $\{1^m\}$. With this the single particle creation operators $a^\dagger_{j_\alpha m_\alpha}$ belong to $\{1\}$ and the destruction operators $a_{j_\beta m_\beta}$ belong to $\left\{1^{N-1}\right\}$. The only scalar operator in m-particle space is number operator n as it remains invariant under the transformation produced by the generators of $U(N)$ group. One can in general seek a decomposition of a given operator into tensor operators (belonging to a definite irrep of $U(N)$) with respect to $U(N)$ group similar to what one does with respect to $O(3)$ in angular momentum algebra. The tensor decomposition is illustrated below with examples that are relevant for the results given in Chapters 3 - 6.

Let us begin with a NIP hamiltonian $h = \sum \epsilon_\alpha n_\alpha$; ϵ_α are single particle

energies (SPE) and as stated before n_α is number operator for the spherical α. From the above discussions it should be clear that the scalar part h^0 of h with respect to $U(N)$ should be a first order polynomial in number operator n. Then one-body nature of h gives $h^0 = a_0 + a_1 n$. Now taking trace on both sides over 0 and 1-particle spaces immediately gives the result that $h^0 = \langle h \rangle^1 n$. The remaining piece $h^1 = h - h^0$ is the unitary one-body part of h and it has a definite group theoretical meaning in trems of the $U(N)$ group. Thus the unitary decompositon of h is,

$$\begin{aligned} h &= \sum_\alpha \epsilon_\alpha n_\alpha = h^0 + h^1 \\ h^0 &= \sum_\alpha \bar{\epsilon} n_\alpha = \bar{\epsilon} n \; ; \; \bar{\epsilon} = N^{-1} \sum_\alpha \epsilon_\alpha N_\alpha \, , \, n = \sum n_\alpha \\ h^1 &= h - h^0 = \sum_\alpha \epsilon^1_\alpha n_\alpha = \sum \tilde{\epsilon}_\alpha n_\alpha \; ; \; \epsilon^1_\alpha = \tilde{\epsilon}_\alpha = \epsilon_\alpha - \bar{\epsilon} \end{aligned} \tag{2.49}$$

Note that in the remainder of the thesis $\tilde{\epsilon}_\alpha$ and ϵ^1_α are used interchangeably when there is no confusion; some time $\epsilon^1_\alpha(1)$ is used to emphasize that the SPE are derived from a one-body hamiltonian. Unitary decomposition of a two-body interaction V defined by the two-body matrix elements (TBME) $V^J_{\alpha\beta\gamma\delta}$ is easy to work out in terms of the average two-particle matrix elements $V_{\alpha\beta}$,

$$V_{\alpha\beta} = \left\{ \check{N}_{\alpha\beta} \right\}^{-1} \left\{ \sum_J [J] V^J_{\alpha\beta\alpha\beta} \right\} = \{ N_{\alpha\beta} \}^{-1} \left\{ \sum_J [J] V^J_{\alpha\beta\alpha\beta} (1 + \delta_{\alpha\beta}) \right\} . \tag{2.50}$$

In (2.50), $[J] = (2J + 1)$. Recognizing that the scalar part V^0 of V with respect to $U(N)$ group should be a second order polynomial in n gives the result $V^0 = a_0 + a_1 n + a_2 n^2$. Once again taking the traces over 0, 1 and 2-particle spaces on both sides of the above equation leads to the following simple formula for V^0,

$$\begin{aligned} V^0 &= \binom{n}{2} \langle V \rangle^2 = \binom{n}{2} \bar{V} = [n]_2 [N]_2^{-1} \left[\sum_{\alpha \geq \beta} \check{N}_{\alpha\beta} V_{\alpha\beta} \right] \\ &= [n]_2 [N]_2^{-1} \left[\frac{1}{2} \sum_{\alpha,\beta} N_{\alpha\beta} V_{\alpha\beta} \right] \end{aligned} \tag{2.51}$$

Just as h has h^1 part, V should have a one-body part with respect to $U(N)$ group. This part which is denoted as V^1, should vanish in 0 and 1-particle spaces. Therefore the form of V^1 is $V^1 = (n-1)F^1 = (n-1)\sum \epsilon^1_\alpha(2) n_\alpha$. Then, $V - V^0 = V^1 + V^2$; it should be obvious that the V^2 part cannot be reduced to a piece that behaves as neither V^0 nor V^1. The explicit forms of F^1 and V^2 are derived by using the particle-hole (p-h) symmetries of these operators, $F^1 \overset{p-h}{\longrightarrow} -F^1$ and $V^2 \overset{p-h}{\longrightarrow} V^2$. This gives the results

$$\begin{aligned} V^1 &= (n-1)\sum \epsilon^1_\alpha(2) n_\alpha \overset{\substack{For\ m \\ particles}}{\longrightarrow} \sum_\alpha \zeta^1_\alpha(m) n_\alpha \ , \\ V^2 &= V - V^0 - V^1 \ ; \\ \zeta^1_\alpha(m) &= (m-1)\epsilon^1_\alpha(2) \\ \epsilon^1_\alpha(2) &= (N-2)^{-1} \sum_\gamma (N_\gamma - \delta_{\alpha\gamma})(V_{\alpha\gamma} - (V)^2) \end{aligned} \tag{2.52}$$

Eqs. (2.49) - (2.52) give the unitary decomposition of $V = \sum_{\nu=0,1,2} V^\nu$ of V with respect to $U(N)$ group. It is obvious that V^0 is scalar with respect to $U(N)$ (hence denoted as $\nu = 0$ part) , V^1 is effective one-body operator with respect to $U(N)$ as n behaves as a constant when acted on a $U(N)$ irrep $\{1^m\}$ (hence denoted as $\nu = 1$ part) and the remaining piece must be an irreducible two-body part (hence denoted as $\nu = 2$ part); for details regarding Young columnar shapes associated with each ν, see [Ch-71]. Combining the decompositions given by (2.49) - (2.52) one has the following pictorial representation for $U(N)$ decomposition of a one plus two-body hamiltonian $H = h(1) + V(2)$,

$$
\begin{array}{ccccc}
H & = & h(1) & + & V(2) \\
 & & \swarrow\ \searrow & & \swarrow\ \downarrow\ \searrow \\
 & & h^0 + h^1 & & V^0 + V^1 + V^2 \\
 & & \searrow\ \swarrow & & \swarrow\ \searrow \\
 & & H^0 & + H^1 + & H^2
\end{array}
\tag{2.53}
$$

In m-particle space, $H^0 = m\bar{\epsilon} + \begin{pmatrix} m \\ 2 \end{pmatrix} \bar{V}$ while H^1 is defined by m - dependent s.p. energies $\xi^1_\alpha(m)$,

$$
\begin{aligned}
H^1 &= \sum \{\epsilon^1_\alpha(1) + \zeta^1_\alpha(m)\} n_\alpha = \sum_\alpha \xi^1_\alpha(m) n_\alpha ; \\
\xi^1_\alpha(m) &= \epsilon^1_\alpha(1) + (m-1)\epsilon^1_\alpha(2)
\end{aligned}
\tag{2.54}
$$

In (2.54), $\epsilon^1_\alpha(2)$ are the (defined by (2.52)) induced (by V) s.p. energies and $\xi^1_\alpha(m)$ are the renormalized (by V) s.p. energies.

2.5.2 Spherical configuration group $U(N_\alpha) \oplus U(N_\beta) \oplus .....$

The unitary group $U(N_\alpha)$ acting in each spherical orbit α generates m_α of spherical configurations $\mathbf{m}$; i.e. $\mathbf{m}$ behaves as $\{1^{m_\alpha}\} \otimes \{1^{m_\beta}\} \otimes .....$ with respect to the direct sum group $U(N_\alpha) \oplus U(N_\beta) \oplus .....$ Thus in the spherical configurations space, the scalar operators are n_α's. Therefore it should be obvious that the NIP hamiltonian h is a scalar with respect to the spherical configuration group,

$$
h = \sum \epsilon_\alpha n_\alpha = h^{[0]}. \tag{2.55}
$$

In (2.55) $h^{[0]} = h^{[0,0,\cdots]}$ denotes that it is a scalar with respect to each spherical orbit. In order to extract out $V^{[0]}$ the scalar part of V with respect to spherical configurations, it should be recognized that $V^{[0]}$ must be a second order

polynomial in n_α's. Therefore $V^{[0]} = a_0 + \sum_\alpha b_\alpha n_\alpha + \sum_{\alpha \geq \beta} C_{\alpha\beta} \check{n}_{\alpha\beta}$ and then taking traces on both sides in 0, 1 and 2-particle spaces, one has the result

$$V^{[0]} = \sum_{\alpha \geq \beta} V_{\alpha\beta} \check{n}_{\alpha\beta} = \frac{1}{2} \sum_{\alpha,\beta} V_{\alpha\beta} n_{\alpha\beta} \tag{2.56}$$

As a one-body hamiltonian will be a scalar with respect to spherical configuration group (see [Ch-71] for exceptions), there cannot be an effective one-body part of V with respect to spherical configuration group. Thus $\mathbf{V} = V - V^{[0]}$ should be like the $\nu = 2$ part $V^{\nu=2}$ introduced in the $U(N)$ case. Just as $V^{[0]}$ is scalar with respect to each of the $U(N_\alpha)$ groups (therefore the notation $[0] = [0, 0, ...]$), $\mathbf{V}$ behaves as $[2] = (\nu_\alpha, \nu_\beta, ...)$; $\sum \nu_\alpha = 2$. The exact definitions of ν_α's and the methods for enumerating and constructing the various $V^{(\nu_\alpha, \nu_\beta, ...)}$; $\sum \nu_\alpha = 2$, are given by Chang et al [Ch-71]. It suffices for the results presented in Chapters 3 - 6 to mention that $\mathbf{V}$ behaves as [2];

$$\mathbf{V} = V^{[2]} = V - V^{[0]} \tag{2.57}$$

It is important to point out that the tensorial nature of $\mathbf{V}$ with respect to $U(N)$ is exactly $\nu = 2$, i.e. $\mathbf{V} \rightarrow \mathbf{V}^{\nu=2}$ and $\mathbf{V}^{\nu=0} = 0$ and $\mathbf{V}^{\nu=1} = 0$.

2.5.3 Unitary configuration group $U(N_\alpha) \oplus U(N_\beta) \oplus .....$

The unitary group $U(N_{\boldsymbol{\alpha}})$ acting in each unitary orbit $\boldsymbol{\alpha}$ generates $m_{\boldsymbol{\alpha}}$ of a unitary configuration [m]; i.e. [m] behaves as $\{1^m \boldsymbol{\alpha}\} \otimes \left\{1^{m} \boldsymbol{\beta}\right\} \otimes .....$ with respect to the direct sum group $U(N_{\boldsymbol{\alpha}}) \oplus U(N_{\boldsymbol{\beta}}) \oplus .....$ Thus in the unitary configurations space, the scalar operators are $m_{\boldsymbol{\alpha}}$'s. One can carry out decomposition of $H = h(1) + V(2)$ with respect to the group $U(N_{\boldsymbol{\alpha}}) \oplus U(N_{\boldsymbol{\beta}}) \oplus ....$ However the only decomposition is of relevance for present thesis is the decomposition of $h^{[0]} + V^{[0]}$. They will have $[\mathbf{0}] \oplus [\mathbf{1}] \oplus [\mathbf{2}]$ tensor parts with respect

to the above direct sum group and these various tensor parts are obtained as follows.

Given a general one plus two-body operator $A = B(1) + C(2)$ [1] defined by the SPE $\mathcal{E}_\alpha$ and TBME $C^J_{\alpha\beta\gamma\delta}$, $B = \sum \mathcal{E}_\alpha n_\alpha$ and the two-body operator C relevant for the present discussion is described by the average two-particle matrix elements $C_{\alpha\beta}$, $C \Leftrightarrow C_{\alpha\beta} = \check{N}^{-1}_{\alpha\beta}\left[\sum_J [J] C^J_{\alpha\beta\alpha\beta}\right]$. It should be noted that $B = B^{[0]} + B^{[1]}$, $C = C^{[0]} + C^{[1]} + C^{[2]}$ and $A = A^{[0]} + A^{[1]} + A^{[2]}$; $A^{[0]} = B^{[0]} + C^{[0]}$, $A^{[1]} = B^{[1]} + C^{[1]}$ and $A^{[2]} = C^{[2]}$. The explicit expressions for $B^{[\nu]}$, $C^{[\nu]}$ and $A^{[\nu]}$ are derived using the results [Fr-89a]: (i) $\boldsymbol{\nu} = [\nu_{\boldsymbol{\alpha}}, \nu_{\boldsymbol{\beta}}, ...]$, $\sum \nu_{\boldsymbol{\alpha}} = \boldsymbol{\nu}$ and $\nu_{\boldsymbol{\alpha}}$ are integers; (ii) the part that behaves as, $[\mathbf{0}] = [0, 0, ...]$ should be a polynomial in $m_{\boldsymbol{\alpha}}$ (first order for $B^{[0]}$ and second order for $C^{[0]}$); (iii) subtraction of $B^{[0]}$ from B gives $B^{[1]}$; (iv) the $C^{[1]}$ part of $C_{\alpha\beta}$ term with α and β belonging to the same $\boldsymbol{\alpha}$, follows directly from (2.52) and in the case where α and β belong to different unitary orbits, one has to change the $(m-1)$ factor in (2.52) to $m_{\boldsymbol{\alpha}}$ and $m_{\boldsymbol{\beta}}$ appropriately. The final results are,

$$B^{[\mathbf{0}]} = \sum_{\boldsymbol{\alpha}} [\mathcal{E}_{\boldsymbol{\alpha}}(A)] n_{\boldsymbol{\alpha}} \quad ; \quad \mathcal{E}_{\boldsymbol{\alpha}}(A) = \left(\sum_{\alpha \in \boldsymbol{\alpha}} \mathcal{E}_\alpha N_\alpha\right) N^{-1}_{\boldsymbol{\alpha}}$$

$$B^{[1]} = \sum [\mathcal{E}^{[1]}_\alpha(A)] n_\alpha \quad ; \quad \mathcal{E}^{[1]}_\alpha(A) = \mathcal{E}_\alpha - [\mathcal{E}_{\boldsymbol{\alpha}}(A)]$$

$$C^{[\mathbf{0}]} \Leftrightarrow C_{\boldsymbol{\alpha\beta}}(A) = \left[\sum_{\alpha \in \boldsymbol{\alpha}, \beta \in \boldsymbol{\beta}} N_{\alpha\beta} C_{\alpha\beta}\right] \left[N_{\boldsymbol{\alpha\beta}}\right]^{-1}$$

[1] General notations are used here for one plus two-body operator. This is because, the unitary decomposition results of this section are used in Chapter 5 ahead where the one plus two-body operator does not come from a hamiltonian but it derives for example from a transition operator. Unitary decomposition being a group decomposition, it applies for any one plus two-body operator. In terms of these general notations different parts of the hamiltonian H are $H \equiv A$, $h(1) \equiv B(1)$ and $V(2) \equiv C(2)$.

$$
\begin{aligned}
& C^{[1]} \Leftrightarrow \mathcal{E}_{\alpha}^{[1];\boldsymbol{\beta}}(A) \\
& = \left\{ \left[\sum_{\beta \in \boldsymbol{\beta}} (N_{\beta} - \delta_{\alpha\beta}) C_{\alpha\beta} \right] - (N_{\boldsymbol{\beta}} - \delta_{\boldsymbol{\alpha\beta}}) C_{\boldsymbol{\alpha\beta}} \right\} \times \{ N_{\boldsymbol{\beta}} - 2\delta_{\boldsymbol{\alpha\beta}} \}^{-1} \\
& C^{[2]} \Leftrightarrow C_{\alpha\beta}^{[2]}(A) = C_{\alpha\beta} - [C_{\boldsymbol{\alpha\beta}}(A)] - \left\{ \left[\mathcal{E}_{\alpha}^{[1];\boldsymbol{\beta}}(A) \right] + \left[\mathcal{E}_{\beta}^{[1];\boldsymbol{\alpha}}(A) \right] \right\} \\
& A^{[0]} = \sum_{\boldsymbol{\alpha}} [\mathcal{E}_{\boldsymbol{\alpha}}(A)]\, n_{\boldsymbol{\alpha}} + \sum_{\boldsymbol{\alpha} \geq \boldsymbol{\beta}} [C_{\boldsymbol{\alpha\beta}}(A)] \check{n}_{\boldsymbol{\alpha\beta}} \\
& A^{[1]} = \sum_{\alpha} \left\{ \left[\mathcal{E}_{\alpha}^{[1]}(A) \right] + \sum_{\boldsymbol{\beta}} (n_{\boldsymbol{\beta}} - \delta_{\boldsymbol{\alpha\beta}}) \left[\mathcal{E}_{\alpha}^{[1];\boldsymbol{\beta}}(A) \right] \right\} n_{\alpha} \\
& \xrightarrow{\text{for a [m]}} \sum_{\alpha} \xi_{\alpha}^{1}([\mathrm{m}] : A) n_{\alpha} \; ; \\
& \xi_{\alpha}^{1}([\mathrm{m}] : A) = \mathcal{E}_{\alpha}^{[1]}(A) + \zeta_{\alpha}^{[1]}([\mathrm{m}] : A) \; , \\
& \zeta_{\alpha}^{[1]}([\mathrm{m}] : A) = \sum_{\beta} (m_{\beta} - \delta_{\boldsymbol{\alpha\beta}}) \mathcal{E}_{\alpha}^{[1];\boldsymbol{\beta}}(A) \\
& A^{[2]} \Leftrightarrow C_{\alpha\beta}^{[2]}(A)
\end{aligned}
\tag{2.58}
$$

Just as the case with (2.54), $\zeta_{\alpha}^{1}([\mathrm{m}])$ are the induced SPE and $\xi_{\alpha}^{[1]}([\mathrm{m}])$ are the renormalized SPE (for a fixed unitary configuration [m]). In the case of $H^{[0]} = h^{[0]} + V^{[0]}$ decomposition $A = H^{[0]}$, $B = h^{[0]}$ and $C = V^{[0]}$ in (2.58). It is useful to point out that $\mathbf{V}$ given in (2.57) is $V^{[2]}$ type with respect to the unitary configurations, i.e. $\mathbf{V}^{[0]} = 0$, $\mathbf{V}^{[1]} = 0$ and it should be recognized that the $\nu_{\boldsymbol{\alpha}}$ of [2] in $\mathbf{V}^{[2]}$ need not be integers (they can be half integers) [Ch-71].

2.6 Trace propagation

2.6.1 $U(N)$ group averages

Given a m-particle space generated by distributing the particles in N s.p. states the $U(N)$ (or scalar) trace ($\sum_{\alpha \in m} \langle m_{\alpha} | \mathcal{O} | m_{\alpha} \rangle$) of an operator $\mathcal{O}$ over the

entire m-particle space propagates from the corresponding traces in few particle spaces, i.e. the trace will be a polynomial in particle number m with the expansion coefficients determined by the basic few particle (or input) traces. The general principles of $U(N)$ or scalar trace (the word trace and average are used synonymously) propagation are described below with examples that are relevant for the thesis.

i) The trace $\langle F(K)\rangle^m$ of a K-body operator $F(K)$ over the m-particle space is nothing but the trace over the space defined by $\{1^m\}$ of $U(N)$. As traces are invariant under unitary transformations, the trace equivalent operator in the $U(N)$ case of interest should be a function of the invariant operators of $U(N)$. In the scalar case the only invariant operator is the number operator n and therefore one has the elementary result

$$\langle F(K)\rangle^m = \begin{pmatrix} m \\ K \end{pmatrix} \langle F(K)\rangle^K \tag{2.59}$$

which shows that the m-particle average propagates from the defining K-particle average via the binomial $\begin{pmatrix} m \\ K \end{pmatrix}$. A simple application of (2.59) is writing down the m-particle average of h defined by the SPE ϵ_α's and V defined by the TBME $V^J_{\alpha\beta\gamma\delta}$,

$$\begin{aligned} \langle h\rangle^m &= m\langle h\rangle^1 = \frac{m}{N}\sum_\alpha \epsilon_\alpha N_\alpha = m\bar{\epsilon} \\ \langle V\rangle^m &= \begin{pmatrix} m \\ 2 \end{pmatrix} \langle V\rangle^2 = \begin{pmatrix} m \\ 2 \end{pmatrix} \bar{V} \\ &= [m]_2[N]_2^{-1} \sum_{J,\alpha\geq\beta} [J] V^J_{\alpha\beta\alpha\beta} \end{aligned} \tag{2.60}$$

The $\bar{\epsilon}$ and $\bar{V}$ in (2.60) are defined by (2.49 - 2.51).

ii) Extending (2.59), it is very easy to recognize that the scalar average of a $0+1+2+...+K$-body operator $F(0-K)$ is a K^{th} degree polynomial

in m,

$$\langle F(0-K)\rangle^m = \sum_{r=0}^{K} a_r m_r. \tag{2.61}$$

The $(K+1)$ - inputs a_r's can be written in terms of the averages of $F(0-K)$ for any $(K+1)$ values of m. For example let us consider $\langle \widetilde{H}^2\rangle^m = \langle (H - \langle H\rangle^m)^2\rangle^m = \langle (h - \langle h\rangle^m + V - \langle V\rangle^m)^2\rangle^m$. Now $r = 4$ in (2.61). Solving for a_r's in terms of $\langle \widetilde{H}^2\rangle^m$ with $m = 0, 1, 2, N-1, N$ and recognizing that the averages for $m = 0$, N are zero, gives the result,

$$\langle \widetilde{H}^2\rangle^m = [m]_2[N-m]_2[N-2]_2^{-1} \times$$

$$\left[\tfrac{1}{2}\langle \widetilde{H}^2\rangle^2 - \frac{(N-3)(m-2)}{(N-1)(m-1)}\langle \widetilde{H}^2\rangle^1 + \frac{(m-2)}{(N-1)(N-m-1)}\langle \widetilde{H}^2\rangle^{N-1}\right] \tag{2.62}$$

Alternatively $\langle \widetilde{H}^2\rangle^m$ can be written in terms of averages over $m = 0$, 1, 2, 3, 4 which then would have involved calculation of the input traces over 3 and 4-particle spaces. However as (2.62) shows, by exploiting the properties of the operator under question it is possible to reduce the input traces to a minimal set of easily calculable traces.

iii) There are further simplifications in the choice of the input traces if operators with definite unitary rank are used (unitary decomposition of operators with respect to $U(N)$ is already discussed in Sect. 2.5.1); the simplicity arises from the p-h symmetries of these operators. For example using the unitary decomposition of $h = h^0 + h^1$ as given by (2.49), it is easy to see that the trace of h is completely given by h^0 and for calculating the trace of $(h^1)^2$ a good choice of inputs is the points at $m = 0$ and 1. These immediately give the following propagation equations,

$$\langle h\rangle^m = \langle h^0\rangle^m = m\bar{\epsilon}$$

$$\langle (h^1)^2 \rangle^m = \frac{mm^\times}{[N]_2} \langle (h^1)^2 \rangle^1 \; ; \langle (h^1)^2 \rangle^1 = \frac{\sum (\epsilon^1_\alpha)^2 N_\alpha}{N} \tag{2.63}$$

Using the p-h symmetry $\langle (h^1)^3 \rangle^m = -\langle (h^1)^3 \rangle^{N-m}$ and choosing the inputs to be the values of $\langle (h^1)^3 \rangle^m$ for $m = 0$, N, 1, $N-1$, yield the following propagation equation for $\langle (h^1)^3 \rangle^m$,

$$\begin{aligned} \langle (h^1)^3 \rangle^m &= \frac{mm^\times (m^\times - m)}{[N]_3} \langle (h^1)^3 \rangle^1 \; ; \\ \langle (h^1)^3 \rangle^1 &= \frac{\sum (\epsilon^1_\alpha)^3 N_\alpha}{N} \end{aligned} \tag{2.64}$$

Similarly the propagation equation for $\langle (V^{\nu=2})^2 \rangle^m$ is derived by using the p-h symmetry $\langle (V^{\nu=2})^2 \rangle^m = \langle (V^{\nu=2})^2 \rangle^{N-m}$. Choosing the input points for $m = 0, 1, 2, N, N-1$ and the property $\langle (V^{\nu=2})^2 \rangle^m = 0$ for $m = 0$, 1, N, $N-1$, the final result in terms of the TBME $V^J_{\alpha\beta\gamma\delta}(\nu = 2)$ of $V^{\nu=2}$ is

$$\begin{aligned} \langle (V^{\nu=2})^2 \rangle^m = \frac{[m]_2 [m^\times]_2}{[N]_4} \times \\ \sum_{\alpha \geq \beta, \gamma \geq \delta, J} [J] (V^J_{\alpha\beta\gamma\delta}(\nu = 2))^2. \end{aligned} \tag{2.65}$$

Using the unitary decomposition of h and V as given by (2.49) - (2.52) and using the propagation equations of $(h^1)^2$ and $(V^{\nu=2})^2$ given by (2.63) and (2.65), an explicit expression (unlike what is given by (2.65)) for $\langle \widetilde{H^2} \rangle^m$ is,

$$\begin{aligned} \langle \widetilde{H^2} \rangle^m &= \frac{mm^\times}{[N]_2} \left[\sum_\alpha (\epsilon^1_\alpha + (m-1)\epsilon^1_\alpha(2))^2 N_\alpha \right] \\ &+ \frac{[m]_2 [m^\times]_2}{[N]_4} \sum_{\alpha \geq \beta, \gamma \geq \delta, J} [J] (V^J_{\alpha\beta\gamma\delta}(\nu = 2))^2. \end{aligned} \tag{2.66}$$

(iv) In general it is possible to combine the principles involved in (i) - (iii) to derive simple propagation equations in some complicated examples. For example, in evaluating $\langle (h^1)^P \rangle^m$ for $P = 4$ and 5 one needs to extract

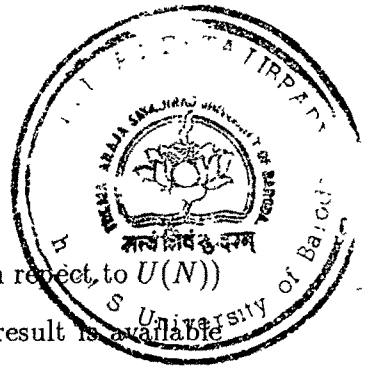
only the one and two-body parts of $(h^1)^P$ denoted as $X_P(i)$, $i = 1, 2$. The unitary tensor nature of h^1 and p-h symmetry will allow us to write $\langle (h^1)^P)^m$ as $p_1(m)X_P(1) + p_2(m)X_P(2)$ and the polynomials p_1 and p_2 are easily determined using (i) and (ii). Then the propagation equation for $\langle (h^1)^4)^m$ is

$$\langle (h^1)^4)^m = \frac{mm^{\times}N}{[N]_4}\left\{\left[N(N+1) - 6mm^{\times}\right]\left[N^{-1}\sum_{\alpha}(\epsilon^1_{\alpha})^4 N_{\alpha}\right] + 3(m-1)(m^{\times}-1)N\left[N^{-1}\sum_{\alpha}(\epsilon^1_{\alpha})^2 N_{\alpha}\right]^2\right\} \quad (2.67)$$

Similarly for $\langle (h^1)^6)^m$ one needs to extract out $X_6(i)$, $i = 1, 2, 3$. An equally simple case is the propagation equation for $\langle h^1(V^{\nu=2})^2)^m$ and one needs here the input trace over 2-particle space and the final result is

$$\langle h^1(V^{\nu=2})^2)^m = \frac{[m]_2[m^{\times}]_2(m^{\times}-m)}{[N]_5}\times \frac{1}{2}\sum_{rtuv}[J]\epsilon^1_r(V^J_{rtuv}(\nu=2))^2(1+\delta_{rt})(1+\delta_{uv}). \quad (2.68)$$

(v) The elementary traces of basic one to three-body operators in $1-3$ - particle spaces are: $\langle (a^{\dagger}_A a_B)\rangle^1 = \delta_{AB}$; $\langle (a^{\dagger}_A a^{\dagger}_B a_C a_D)\rangle^2 = \delta_{BC}\delta_{AD} - \delta_{AC}\delta_{BD}$; $\langle (a^{\dagger}_A a^{\dagger}_B a^{\dagger}_C a_D a_E a_F)\rangle^3 = \delta_{FA}\delta_{DC}\delta_{EB} - \delta_{FA}\delta_{DB}\delta_{EC} - \delta_{EA}\delta_{DC}\delta_{FB} + \delta_{EA}\delta_{DB}\delta_{FC} + \delta_{DA}\delta_{EC}\delta_{FB} - \delta_{DA}\delta_{EB}\delta_{FC}$, where A, B, C etc. are single particle state indices. Extracting out the definite body rank parts of an operator which is a product of several (say $\nu = 2$) operators is tedious but straight forward. To do this, one has to put the operator in normal order form which follows by applying the anticommutation properties of single fermion state operators; $[a^{\dagger}_A a^{\dagger}_B]_+ = 0$, $[a_A\, a_B]_+ = 0$, $[a_A\, a^{\dagger}_B]_+ = \delta_{AB}$. Applying this together with (i), (ii), (iii) for the $\langle \mathbf{UVW})^m$ trace ($\mathbf{U}$, $\mathbf{V}$ and $\mathbf{W}$ are three different two-body interactions; note that as stated



below (2.57) **U**, **V** and **W** are automatically $\nu = 2$ with respect to $U(N)$) gives (we carried out this exercise although the final result is available in [Ay-74a, Wo-86]) the formula,

$$\langle \mathbf{UVW} \rangle^m = \left[\frac{[m]_3 [m^\times]_3}{[N]_6} \right] \mathbf{A} + \left[\frac{[m]_4 [m^\times]_2}{[N]_6} + \frac{[m]_2 [m^\times]_4}{[N]_6} \right] \mathbf{B}$$

$$\mathbf{A} = \sum_{\substack{\Delta \\ rstuxy}} (-1)^{r-t-\Delta} [\Delta]^{-1/2} \beta^{\Delta}_{rtsu}(\mathbf{U}) \beta^{\Delta}_{xysu}(\mathbf{V}) \beta^{\Delta}_{xytr}(\mathbf{W})$$

$$\mathbf{B} = \frac{1}{8} \sum_{\substack{J \\ \alpha\beta\gamma\delta\phi\psi}} [J] \widetilde{\mathbf{U}}^J_{\alpha\beta\gamma\delta} \widetilde{\mathbf{V}}^J_{\gamma\delta\phi\psi} \widetilde{\mathbf{W}}^J_{\phi\psi\alpha\beta} \; ;$$

$$\beta^{\Delta}_{rtsu}(\mathbf{X}) = \sum_J (-1)^{s+t+J+\Delta} [\Delta]^{1/2} [J] \begin{Bmatrix} r & s & J \\ u & t & \Delta \end{Bmatrix} \widetilde{\mathbf{X}}^J_{rstu}$$

$$\widetilde{\mathbf{X}}^J_{rstu} = \sqrt{(1+\delta_{rs})(1+\delta_{tu})} \mathbf{X}^J_{rstu} \; ; \; \mathbf{X} = \mathbf{U}, \mathbf{V} or \mathbf{W} \qquad (2.69)$$

2.6.2 Spherical configuration averages

The principles used in deriving scalar trace propagation equations apply equally well for configuration traces $\langle F \rangle^{[m]}$ of an operator F. This was done in detail in [Fr-71a, Ch-71, Ay-74a, He-75, Po-75, Pa-78, Wo-86]. However there is a simple method to produce fixed configuration traces [Fr-89a, Fr-89b, Fr-94] of operator products with the operators having fixed unitary rank with respect to the spherical configuration group. To derive the propagation equation for the trace $\langle A^{[\nu_1]} B^{[\nu_2]} .... \rangle^m$ one has to start with the scalar trace propagation formula for $\langle A^{\nu_1} B^{\nu_2} ... \rangle^m$. Then one has to attach appropriate spherical orbit indices to particle number m and degeneracy N in the corresponding scalar propagation formulas and carry out the summation over all the spherical orbit indices after multiplying the propagator with the input with spherical orbit

indices. The input matrix elements of A^{ν_1}, B^{ν_2},... etc. are to be replaced by the matrix elements of $A^{[\nu_1]}$, $B^{[\nu_2]}$,... respectively. The right correspondence between the indices of inputs and those of propagators is to be decided and this can easily be done with a computer program. Simple examples are $\langle h\rangle^{\mathbf{m}} = \sum \epsilon_\alpha m_\alpha$ and $\langle V\rangle^{\mathbf{m}} = \sum_{\alpha\leq\beta} V_{\alpha\beta}\check{m}_{\alpha\beta}$ and they follow from (2.60) as $\langle h\rangle^{\mathbf{m}} = \langle h^{[0]}\rangle^{\mathbf{m}}$ and $\langle V\rangle^{\mathbf{m}} = \langle V^{[0]}\rangle^{\mathbf{m}}$. Propagation equation for $\langle \mathbf{V}^2\rangle^{\mathbf{m}}$ is easily obtained by starting with (2.65), changing $[m]_2 = m(m-1)$ by $m_{\alpha\beta}$ and $[m^{\mathrm{x}}]_2$ by $m^{\mathrm{x}}_{\alpha\beta}$ and noting that $\mathbf{V} = \mathbf{V}^{[2]}$. Thus for the traces $\langle \mathbf{UV}\rangle^{\mathbf{m}}$ or $\langle \mathbf{V}^2\rangle^{\mathbf{m}}$, ($\mathbf{U}$, $\mathbf{V}$ are of $\nu = [2]$ type with respect to spherical configuration group) it is easy to recognize the right combination of the indices in the propagators and the inputs,

$$\langle \mathbf{UV}\rangle^{\mathbf{m}} = \sum_{\substack{\alpha,\beta\\ \gamma,\delta}} m_{\alpha\beta}m^{\mathrm{x}}_{\gamma\delta}\left[N_{\alpha\beta\gamma\delta}\right]^{-1}\left\{\frac{1}{4}\sum_J [J]\mathbf{U}^J_{\alpha\beta\gamma\delta}\mathbf{V}^J_{\alpha\beta\gamma\delta}(1+\delta_{\alpha\beta})(1+\delta_{\gamma\delta})\right\} \tag{2.70}$$

The trace $\langle h^{[1]}\mathbf{V}^2\rangle^{\mathbf{m}}$ is zero because $h^{[1]}$ is zero. Using the method described above, it is possible to write down the formula for $\langle \mathbf{UVW}\rangle^{\mathbf{m}}$ using (2.69). The explicit formula is given in [Wo-86].

2.6.3 Unitary configuration averages

For unitary configuration traces $\langle F\rangle^{[\mathbf{m}]}$ the same procedure as above can be adopted (after carrying out tensorial decomposition of the operators involved with respect to the unitary configuration group). In this case unitary orbit indices are to be attached with m, N etc. of the propagators of the corresponding scalar trace propagation formulas and the summation is now over all unitary orbit indices. For the inputs, the indices are spherical orbit indices that belong

to particular unitary orbits and then the summation over those spherical orbit indices are to be carried out. Like in the spherical configurations case, the right combination of indices in the propagators and the inputs can be found out using a computer program. The formulas for $\langle \mathbf{UV} \rangle^{[\mathbf{m}]}$, $\langle h^{[1]}(\mathbf{V})^2 \rangle^{[\mathbf{m}]}$ and $\langle \mathbf{UVW} \rangle^{[\mathbf{m}]}$ are given below.

The derivation of trace propagation formula for $\langle \mathbf{UV} \rangle^{[\mathbf{m}]}$ is straight forward as $\mathbf{U}$ and $\mathbf{V}$ both have unitary rank [2] as stated below (2.58). Using the scalar result (2.65) (and also (2.70)) the formula for $\langle \mathbf{UV} \rangle^{[\mathbf{m}]}$ can be written down,

$$\begin{aligned} \langle \mathbf{UV} \rangle^{[\mathbf{m}]} \;=\; & \sum_{\mathbf{r,s,t,u}} \left[m_{\mathbf{rs}} m^{\times}_{\mathbf{tu}} \right] (N_{\mathbf{rstu}})^{-1} \times \\ & \frac{1}{4} \sum_{J} [J] \mathbf{U}^{J}_{rstu} \mathbf{V}^{J}_{rstu} (1+\delta_{rs})(1+\delta_{tu}) \\ & \quad r \in \mathbf{r},\, s \in \mathbf{s} \\ & \quad t \in \mathbf{t},\, u \in \mathbf{u} \end{aligned} \tag{2.71}$$

The formula for $\langle (h^{\mathbf{1}})\mathbf{V}^{\mathbf{2}} \rangle^{[\mathbf{m}]}$ (required to calculate spin-cutoff density variance) is derived using the scalar result (2.68) and then looking for the correct combination of indices with the help of a computer program [Ha-92, Fr-94],

$$\begin{aligned} \langle (h)^{[\mathbf{1}]}(\mathbf{V})^{\mathbf{2}} \rangle^{[\mathbf{m}]} \;=\; & \sum_{\mathbf{r,t,u,v}} \left[N^{-1}_{\mathbf{rtuvr}} m_{\mathbf{rt}} m^{\times}_{\mathbf{uvr}} - N^{-1}_{\mathbf{uvrrt}} m_{\mathbf{uvr}} m^{\times}_{\mathbf{tr}} \right] \times \\ & \frac{1}{2} \sum_{J} [J] \epsilon^{[\mathbf{1}]}_{r} \mathbf{V}^{J}_{rtuv} \mathbf{V}^{J}_{uvrt} (1+\delta_{rt})(1+\delta_{uv}) \\ & \quad r \in \mathbf{r}, t \in \mathbf{t} \\ & \quad u \in \mathbf{u}, v \in \mathbf{v} \end{aligned} \tag{2.72}$$

The trace propagation formula for $\langle \mathbf{UVW} \rangle^{[\mathbf{m}]}$ where all $\mathbf{U}$, $\mathbf{V}$, $\mathbf{W}$ are of tensorial rank [2] with respect to unitary configuration group, follows from (2.69) and the expression for $\langle \mathbf{UVW} \rangle^{\mathbf{m}}$ given in [Wo-86]. The final result is

[Ha-92, Fr-94],

$$\langle \mathbf{UVW} \rangle^{[\mathrm{m}]} = \sum_{\substack{\mathbf{r,s,t,u} \\ \mathbf{x,y}}} \left[\left\{ m_{\mathbf{rsy}} m^{\times}_{\mathbf{tux}} N^{-1}_{\mathbf{rsytux}} \right\} \mathbf{A}_{\mathbf{r,s,t,u,x,y}} \right] + \left[\left\{ [m_{\mathbf{rs}} m^{\times}_{\mathbf{tuxy}} N^{-1}_{\mathbf{rstuxy}} + m_{\mathbf{xytu}} m^{\times}_{\mathbf{rs}} \times N^{-1}_{\mathbf{xyturs}} \right\} \mathbf{B}_{\mathbf{r,s,t,u,x,y}} \right]$$

$$\mathbf{A}_{\mathbf{r,s,t,u,x,y}} = \sum_{\substack{\Delta \\ r \in \mathbf{r}, s \in \mathbf{s} \\ t \in \mathbf{t}, u \in \mathbf{u} \\ x \in \mathbf{x}, y \in \mathbf{y}}} (-1)^{r-t-\Delta} [\Delta]^{-1/2} \beta^{\Delta}_{rtsu}(\mathbf{U}) \beta^{\Delta}_{xysu}(\mathbf{V}) \beta^{\Delta}_{xytr}(\mathbf{W})$$

$$\mathbf{B}_{\mathbf{r,s,t,u,x,y}} = \frac{1}{8} \sum_{\substack{J \\ r \in \mathbf{r}, s \in \mathbf{s} \\ t \in \mathbf{t}, u \in \mathbf{u} \\ x \in \mathbf{x}, y \in \mathbf{y}}} [J] \mathbf{U}^{J}_{rstu} \mathbf{V}^{J}_{tuxy} \mathbf{W}^{J}_{xyrs} (1+\delta_{rs})(1+\delta_{tu})(1+\delta_{xy})$$

(2.73)

The definition of the multipole coefficient β^{Δ}_{rstu} appearing in (2.73) is given in (2.69) and it follows from [Fr-66]. The formulas given in (2.71) - (2.73) are used in Chapters 3, 4 and 6. For example the variance $\langle \mathbf{V}^2 \rangle^{[\mathrm{m}]}$ of the density $\rho^{\mathbf{V},[\mathrm{m}]}_{\mathcal{G}}(x) = \langle \delta(\mathbf{V}-x) \rangle^{[\mathrm{m}]}$ follows from (2.71). Similarly the centroids and variances of the spin-cutoff density $\rho^{\mathbf{V},[\mathrm{m}]}_{J^2_Z} = \langle J^2_Z \delta(\mathbf{V}-x) \rangle^{[\mathrm{m}]} / \langle J^2_Z \rangle^{[\mathrm{m}]}$ follow from (2.71 - 2.73). The centroid of the J^2_Z - density derives from the trace $\langle J^2_Z \mathbf{V} \rangle^{[\mathrm{m}]}$ $= \langle (J^2_Z)^{[2]} \mathbf{V} \rangle^{[\mathrm{m}]}$ (since $\langle \mathbf{V} \rangle^{[\mathrm{m}]} = 0$ and $\langle (J^2_Z)^{[1]} \mathbf{V} \rangle^{[\mathrm{m}]} = 0$) and $\langle (J^2_Z)^{[2]} \mathbf{V} \rangle^{[\mathrm{m}]}$ follows from Eq. (2.71). The spin-cutoff density variance derives from the trace $\langle J^2_Z \mathbf{V}^2 \rangle^{[\mathrm{m}]} = \langle (J^2_Z)^{[0]} \mathbf{V}^2 \rangle^{[\mathrm{m}]} + \langle (J^2_Z)^{[1]} \mathbf{V}^2 \rangle^{[\mathrm{m}]} + \langle (J^2_Z)^{[2]} \mathbf{V}^2 \rangle^{[\mathrm{m}]}$ and the three averages on R.H.S. follow from (2.71), (2.72) and (2.73) respectively.

2.7 Summary

Extension and application of the CLT results given in Sect. 2.3 to indefinitely large shell model spaces is the aim of SAT-LSS. This is achieved by using the unitary decompositions of operators described in Sect. 2.5 together with the S - decomposition, introduced ahead in Chapter 3, via spherical and unitary configuration partitioning (Sect. 2.4) and it is made practical by the trace propagation formulas given in Sect. 2.6. It is useful to mention that programs are available [Ko-84b, Ha-92] for carrying out unitary decompositions given in Sect. 2.5 and for the trace propagation formulas given in Sect. 2.6. In the next chapter the basic convolution result for state densities in SAT-LSS is described briefly before turning to a study (and tests) of two important aspects of SAT-LSS. The trace propagation methods described in Sect. 2.6 are used extensively in Chapter 5 to derive large number of trace propagation formulas relevant for the construction of non-interacting particle strength densities.