

a. The “LIT equation”

$$\left( \hat{H}_{\text{nuclear}} - \underbrace{E_0 - \mathcal{R}[\sigma] - i \mathcal{G}[\sigma]}_{:= -\mathcal{E}} \right) \Psi_{\text{LIT}}^{J^\pi m_j} = \left[ \hat{\mathcal{O}}_{Lm_L} \{ |\mathbf{k}|, \mathbf{j}_v \} \otimes \Psi_0^{J_0^{\pi_0}} \right]^{J^\pi m_j} . \quad (1)$$

with

$$v(\text{ertex}) \in \{ \mathbf{j}_o(\mathbf{x}) = \dots, \mathbf{j}_s(\mathbf{x}) = \dots, \mathbf{j}_{\text{mec}}(\mathbf{x}) = \dots, \dots \} ; \quad (2)$$

b. The variational basis

$$\Psi_{\text{LIT}}^{J^\pi m_j} = \sum_n u_n \phi_n^{J^\pi m_j} . \quad (3)$$

with

$$\phi_n^{J^\pi m_j} \in \left\{ [\xi_{S_n} \otimes \mathcal{Y}_{l_n}(\boldsymbol{\rho})]^{Jm_j} e^{-\gamma_n \boldsymbol{\rho}^2} \mid \gamma \in \mathbb{R}_+, s \in \mathbb{N}^{A-1} + \left(\frac{\mathbb{N}}{2}\right)^{A-2}, l \in \mathbb{N}^{A-1} + \mathbb{N}^{A-2} \right\} \quad (4)$$

c. The matrix form of the “LIT equation”

$$\sum_{s=1}^{N_{\text{LIT}}} \phi_r^{J^\pi m_j} \left( \hat{H}_{\text{nuclear}} - \mathcal{E} \right) \phi_s^{J^\pi m_j} u_s = \sum_{n=1}^{N_0} \sum_{m_L} c_n \underbrace{\langle LJ_0; m_L m_j - m_L \mid Jm_j \rangle}_{\text{Eq.(17)}} \phi_r^{J^\pi m_j} \hat{\mathcal{O}}_{Lm_L} \phi_n^{J_0^{\pi_0}(m_j - m_L)} . \quad (5)$$

with

$$N_{\text{LIT}} : \text{number of basis states used to expand the LIT state, e.g., } \Psi_{\text{LIT}}^{2-} ; \quad (6)$$

$$N_0 \leq N_{\text{LIT}} : \text{number of basis states used to expand the target, e.g., the deuteron; } \quad (7)$$

$$(8)$$

d. The matrix element Reduced matrix elements are used where possible in order to reduce the number of numerical evaluations. The composite structure of the operators (spatial and spin form a scalar) demands a more general version of the Wigner-Eckart theorem (*cf.* [1], Eq.(7.1.5)).

$$\phi_m^{J^\pi m_j} \hat{\mathcal{O}}_{Lm_L} \phi_n^{J_0^{\pi_0} m_{j_0}} := \langle m; l_l S_l J_l m_{j_l} \mid \mathcal{A} \mathcal{O}_{Lm_L} \mid l_r S_r J_r m_{j_r}; n \rangle \quad (9)$$

$$= (-1)^{L-J_r+J_l} \underbrace{\langle LJ_r; m_L m_{j_r} \mid J_l m_{j_l} \rangle}_{\text{enemb:600ff}} \underbrace{\langle m; l_l S_l J_l \mid \mathcal{A} \mathcal{O}_L \mid l_r S_r J_r; n \rangle}_{\downarrow} \quad (10)$$

$$\underbrace{\hat{J}_r \hat{J}_l \hat{L} \left\{ \begin{matrix} l_l^m & l_r^n & p \\ S_l^m & S_r^n & q \\ J_l & J_r & L \end{matrix} \right\}}_{\text{enemb:ecce}} \sum_{\text{dc}} \sum_{\mathbf{p} \in \text{dc}} \underbrace{\langle m; l_l^m \mid \mathcal{O}_p^o \mid \mathcal{A}_{\text{dc}} l_r^n; n \rangle}_{\text{luisse}} \cdot \underbrace{\langle m; S_l^m \mid \mathcal{O}_q^s \mid \mathcal{A}_{\mathbf{p}} S_r^n; n \rangle}_{\text{obem}} \quad (11)$$

$$= \hat{J}_r \hat{L} \langle \mathbf{J}_r \mathbf{L}; m_{j_r} m_L \mid J_l m_{j_l} \rangle \cdot \left\{ \begin{matrix} l_l^m & l_r^n & p \\ S_l^m & S_r^n & q \\ J_l & J_r & L \end{matrix} \right\} \quad (12)$$

$$\cdot \sum_{\text{dc}} \sum_{\mathbf{p} \in \text{dc}} \langle m; l_l^m \mid \mathcal{O}_p^o \mid \mathcal{A}_{\text{dc}} l_r^n; n \rangle \cdot \langle m; S_l^m \mid \mathcal{O}_q^s \mid \mathcal{A}_{\mathbf{p}} S_r^n; n \rangle \quad (13)$$

with

$$\hat{a} := \sqrt{2a+1} ; \quad (14)$$

$$\mathcal{A} = \sum_{\mathbf{p} \in \mathcal{S}_{A-1}} (-1)^{\text{sgn}(\mathbf{p})} \hat{\mathbf{p}} = \oplus_{\text{dc}} \quad (15)$$

$$\text{dc} : \text{double co-set} \quad (16)$$

1 *e. The calculation*

(i) Solve

$$\hat{H}_{\text{nuclear}} \Psi^{J_0^{\pi_0}} = E_0 \Psi^{J_0^{\pi_0}}$$

with the ansatz

$$\Psi^{J_0^{\pi_0}} = \sum_n c_n \phi_n^{J_0^{\pi_0}} .$$

2 If  $\hat{H}_{\text{nuclear}}$  is a spherical rank-0 operator – a condition which most practical nuclear potentials satisfy –  
3  $\Psi^{J_0^{\pi_0}} \neq f(m_{j_0})$ . We obtain  $\Psi^{J_0 J_0}$ , in practice.

(ii) Calculate

$$\mathbb{H}_{rs} := \left\langle \phi_r^{J^\pi} \left| \hat{H}_{\text{nuclear}} \right| \phi_s^{J^\pi} \right\rangle \quad \text{and} \quad \mathbb{N}_{rs} := \left\langle \phi_r^{J^\pi} \left| \phi_s^{J^\pi} \right\rangle \quad \forall |L - J_0| \leq J \leq |L + J_0|$$

(iii)  $\forall m_j \& m_L$ , calculate

$$S_{rs, m_L}^{J m_j J_0} := \left\langle \phi_r^{J^\pi m_j} \left| \hat{\mathcal{O}}_{L m_L} \right| \phi_s^{J_0^{\pi_0} J_0} \right\rangle ,$$

4 and superimpose these matrix elements according to Eq.(5)

$$S_r^{J m_j} := \sum_{m_L} \langle L J_0 ; m_L m_j - m_L | J m_j \rangle \underbrace{\sum_n^{N_0} c_n S_{rn, m_L}^{J m_j J_0}}_{\text{enemb.f OUT}} . \quad (17)$$

5 Ecce,  $\Psi^{J_0^{\pi_0}} \neq f(m_{j_0})$  does not allow for an elimination of  $m_j$  from this equation!

6 (iv) Solve the (complex) linear matrix equation

$$(\mathbb{H}_{rs} - \mathbb{E} \mathbb{N}_{rs}) u_s^{J m_j} = S_r^{J m_j} \quad (18)$$

7 to obtain the LIT state

$$\psi_{J_{i(\text{initial})/f(\text{inal}); J_{(i)n(\text{termediate})} m_n}^{v(\text{ertex}), (\text{mu}) L(\text{tipolarity})} (k, \sigma) = \psi_{J_0; J m_j}^{v, L} (k, \sigma) := \Psi_{\text{LIT}}^{J^\pi m_j} \left( \underbrace{|\mathbf{k}|, v, L}_{\text{vertex quantum numbers}} ; \underbrace{E_0, J_0}_{\text{initial/final-state quantum numbers}} ; \mathcal{R}[\sigma], \mathcal{I}[\sigma] \right) . \quad (19)$$

(v) Units exemplified for the  $E1$  calculation:

The units of the LIT ( $\psi$ ) and the ground state ( $\phi$ ) are not identical, in general:

$$\hat{\mathcal{O}}_{\text{nucl}}(\text{MeV}) \psi(x) = \hat{\mathcal{O}}_{\text{E1}}(0) \phi(\text{MeV}^{3/2}) \quad (20)$$

$E1$  is implemented as  $j_1 Y_{1M}$  without any dimensionful prefactors, and hence

$$x = \text{MeV}^{1/2} \Rightarrow [L] = \text{MeV}^{-2} \quad (21)$$

To recover the physical  $E1$ , a factor of

$$\frac{2}{\hbar k} \quad (22)$$

multiplies the RHS.

$$(23)$$

(vi) The inner product

$$\mathcal{L}_{v'L',vL}^{J_f,J_i;J}(k',k,\sigma) = (-1)^{J-J_i+L-L'+v'} N_{J,\sigma} \sum_{m_j} \underbrace{\left\langle \psi_{J_f;Jm_j}^{v',L'}(k',\sigma) \left| \psi_{J_i;Jm_j}^{v,L}(k,\sigma) \right\rangle \right.}_{=\sum_{r,s} (u_r^{Jm_j})^* u_s^{Jm_j} \mathbb{N}_{rs}} \quad (24)$$

$$= \int_{e_{th}}^{\infty} \frac{\mathcal{F}_{v'L',vL}^{J_f,J_i;J}(k',k,\mathbf{E})}{(E-\sigma)(E-\sigma^*)} dE \quad (25)$$

with  $N_{J,\sigma}$  being the multiplicity of Lorentz states for given  $J$  and  $\sigma$ .

(26)

8 (vii) The recovery of the (partial) strength functions – The inverse Lorentz-integral transformation

9 At this stage, the problem is to recover  $\mathcal{F}$ , given  $\mathcal{L}$  by inverting the integral transformation Eq. (25). The  
10 *discrete essence* of that can be written as

$$\mathbf{L}_s = \sum_e A_{se} \mathbf{F}^e = \sum_n c_n \sum_e A_{se} f_n^e . \quad (27)$$

11 If the energy sum/integral can be evaluated efficiently for a set of basis vectors  $f_n$  which is suitable for a  
12 proper representation of the vector  $\mathbf{L}$ , it remains to solve a linear optimization problem. This is detailed  
13 below from Eq. (32) onwards.

14 The choice for the basis  $f_n$  is based on two ideas. Firstly, from the definition

$$\mathcal{F}_{v'L',vL}^{J_f,J_i;J}(k',k,\mathbf{E}) = \underbrace{N_{J,E}}_{\#J,E\text{-states}} \langle J_f E_f || M^{\nu',L'}(k') || J E \rangle \langle J E || M^{\nu,L}(k) || J_i E_i \rangle , \quad (28)$$

15 the joint probability to, first, induce via  $M^{\nu,L}(k)$  the transition from one eigenstate of a system to another,  
16 which, second is perturbed via  $M^{\nu',L'}(k')$  into some final eigenstate. Let me imagine a system with one  
17 localized bound state. Its wave function is folded with the perturbation, which is a polynomial in  $k$  of order  
18  $L$  – the multipolarity – and the wave function of another eigenstate of the system, constrained by energy  
19 conservation. I think of  $k$  large enough such that the latter state contains a free wave on some coordinate.  
20 Hence the matrix element retains a Fourier-transform character of a localized wave packet multiplied by a  
21 polynomial. The latter can be expanded well in symmetrical, peaked functions – *e.g.*, Gaussians – and the  
22 polynomial skews those. A Fourier transform of such a skewed Gaussian will retain its shape but become  
23 broader/narrower. A skewed Gaussian is expected to be amenable to an expansion in Lorentz functions.

24 The second, related idea for choosing a Lorentz basis is the ability to calculate the integral transform with  
25 a Lorentz kernel analytically (viz. Eq. (34)).

(Wigner) 3- $j$  symbol:  $\begin{pmatrix} L & S & J \\ m_l & m_s & -m_j \end{pmatrix} = (-1)^{L-S+m_j} (2J+1)^{-\frac{1}{2}} \langle LS; m_l m_s | J m_j \rangle$  (29)

Matrix for single-axis rotation:  $\mathcal{D}_{m',m}^{(j)}(0 \ \beta \ 0) \equiv d_{m',m}^{(j)}(\beta)$

$$= \left[ \frac{(j+m')!(j-m')!}{(j+m)!(j-m)!} \right]^{\frac{1}{2}} \cdot \sum_{\sigma} \binom{j+m}{j-m'-\sigma} \binom{j-m}{\sigma} (-1)^{j-m'-\sigma} \cdot \left( \cos \frac{\beta}{2} \right)^{2\sigma+m+m'} \left( \sin \frac{\beta}{2} \right)^{2j-2\sigma-m-m'} \quad (30)$$

(31)

27 *a. The Lorentz transformation of a Lorentzian*

28 The strength functions which constitute the Compton amplitudes are themselves composed of scalar functions  
 29 of an energy parameter. I assume that these functions can be expanded to any desired accuracy in a Lorentzian/-  
 30 Cauchy basis as follows:

$$r(e) = \sum_n c_n \frac{\theta(e - e_{\text{th}})}{(a_n - e)^2 + b_n^2} := \sum_n c_n \theta(e - e_{\text{th}}) f_n. \quad (32)$$

31 As the process is non-trivial only if the photon's energy exceeds a minimum threshold energy  $e_{\text{th}}$ , it is in order  
 32 to include a system-characteristic step function.

33 In practice, we obtain an integral transformation of this quantity with a Lorentzian kernel,

$$L(\sigma) := \int_{-\infty}^{\infty} \frac{r(e)}{(\sigma_r - e)^2 + \sigma_i^2} de = \sum_n c_n \int_{e_{\text{th}}}^{\infty} \frac{f_n(e)}{(\sigma_r - e)^2 + \sigma_i^2} de. \quad (33)$$

34 If basis functions<sup>①</sup> which we define through the integral

$$\begin{aligned} \int_{e_{\text{th}}}^{\infty} \frac{f_n(e)}{(\sigma_r - e)^2 + \sigma_i^2} de &= \int_{e_{\text{th}}}^{\infty} \frac{1}{(\sigma_r - e)^2 + \sigma_i^2} \cdot \frac{1}{(a_n - e)^2 + b_n^2} de \\ &\vdots \\ &= [(\sigma_r - a_n)^2 + (\sigma_i - b_n)^2]^{-1} \cdot [(\sigma_r - a_n)^2 + (\sigma_i + b_n)^2]^{-1} \\ &\quad \cdot \left\{ \sigma_i^{-1} ((\sigma_r - a_n)^2 + b_n^2 - \sigma_i^2) \left( \frac{\pi}{2} + \tan^{-1} \left( \frac{\sigma'_r}{\sigma_i} \right) \right) \right. \\ &\quad + b_n^{-1} ((\sigma_r - a_n)^2 - b_n^2 + \sigma_i^2) \left( \frac{\pi}{2} + \tan^{-1} \left( \frac{a'_n}{b_n} \right) \right) \\ &\quad \left. + (\sigma_r - a_n) \ln \left( \frac{\sigma_r'^2 + \sigma_i^2}{a_n'^2 + b_n^2} \right) \right\} \\ &:= L_n(\sigma, e_{\text{th}}) \end{aligned} \quad (34)$$

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<sup>①</sup>  $x' := x - e_{\text{th}}$

$\alpha = \frac{e^2}{4\pi}$	dimensionless	$\frac{1}{137.03604}$
$\hbar c$		197.32858 MeV · fm <sup>2</sup>

TABLE I. Implemented numerical values.

allow for an accurate expansion of a given, physical function  $L(\sigma)$ , namely for a set  $\mathfrak{B} = \{(a_n, b_n) \in \mathbb{R}_{0+}\}_{n=1, \dots, d}$ , we seek

$$\min_{\mathbf{c}} \left| L(\sigma) - \sum_n c_n L_n(\sigma, e_{\text{th}}) \right| := \mathbf{c}^*. \quad (35)$$

The set of optimal parameters  $\mathbf{c}^*$  represents via Eq. (32) an expansion of the response function in Lorentzians. If  $\mathfrak{B}$  is “numerically” complete, the dependence of  $r(e)$  on changes in this basis should be negligible, *i.e.*, the problem is **not** ill-posed. This shall now be demonstrated for an exemplary process.

## II. “HOW TO DO AN INTEGRAL”

### a. The multipole operators

- convection current<sup>①</sup>

$$\mathbf{j}_o(\mathbf{x}) = \frac{e}{2m} \sum_i \frac{1}{2} (1 + \tau_z(i)) \left\{ \mathbf{p}(i), \delta^{(3)}(\mathbf{x} - \mathbf{r}(i)) \right\} \quad (37a)$$

$$\text{(electric)} \quad \mathcal{O}_{Lm_L}^{\text{el}} = \frac{e\hbar}{mc} \hat{L}^{-1} \sum_i g_l(i) \left[ \sqrt{L} \Delta_{LM}^{L+1}(\mathbf{r}(i)) - \sqrt{L+1} \Delta_{LM}^{L-1}(\mathbf{r}(i)) \right] \quad (37b)$$

$$\text{(magnetic)} \quad \mathcal{O}_{Lm_L}^{\text{mag}} = i \frac{e\hbar}{mc} \sum_i g_l(i) \Delta_{LM}^L(\mathbf{r}(i)) \quad (37c)$$

- spin current

$$\mathbf{j}_s(\mathbf{x}) = \frac{e\hbar}{2m} \sum_i \frac{1}{2} (g_{s_p} (1 + \tau_z(i)) + g_{s_n} (1 - \tau_z(i))) \boldsymbol{\sigma}(i) \times \boldsymbol{\nabla}(i) \delta^{(3)}(\mathbf{x} - \mathbf{r}(i)) \quad (38a)$$

$$\text{(electric)} \quad \mathcal{O}_{Lm_L}^{s^{\text{el}}} = - \frac{e\hbar |\mathbf{k}|}{2mc} \sum_i g_s(i) \sum_{M, \nu} \langle L1; M\nu | Lm_L \rangle \cdot \boldsymbol{\sigma}_\nu(i) \Phi_{LM}(\mathbf{r}(i)) \quad (38b)$$

$$\text{(magnetic)} \quad \mathcal{O}_{Lm_L}^{s^{\text{mag}}} = i \frac{e\hbar |\mathbf{k}|}{2mc} \hat{L}^{-1} \sum_i g_s(i) \sum_{M, \nu} \left[ \sqrt{L} \langle L+11; M\nu | Lm_L \rangle \boldsymbol{\sigma}_\nu(i) \Phi_{L+1M}(\mathbf{r}(i)) \right. \quad (38c)$$

$$\left. - \sqrt{L+1} \langle L-11; M\nu | Lm_L \rangle \boldsymbol{\sigma}_\nu(i) \Phi_{L-1M}(\mathbf{r}(i)) \right] \quad (38d)$$

<sup>①</sup>Indices referring to particles are put in brackets.

with

$$\Phi_{Lm_L}(\mathbf{r}) = j_L(kr) Y_{Lm_L}(\Omega_r) \quad \textcircled{1} \quad (39)$$

$$\Delta_{Lm_L}^J(\mathbf{r}) = \sum_{M,\nu} \langle L1; M\nu | Jm_L \rangle \Phi_{Lm_L}(\mathbf{r}) \mathbf{p}_\nu \quad \textcircled{2} \quad (40)$$

<sup>42</sup>

b. *Siegert form* Linear-in- $\alpha$  coupling of a (background) photon (momentum  $\mathbf{k}$ ) to a system ( $j^\nu$ ) at  $\mathbf{x}$ :

$$\left\langle f \left| -\frac{1}{c} \int d\mathbf{x} A_\nu(\mathbf{x}) j^\nu(\mathbf{x}) \right| i \right\rangle \xrightarrow{\text{transverse}} \left\langle f \left| -\sum_{LM} i^L \hat{L} \sqrt{2\pi} (\mathcal{O}_{Lm_L}^{\text{el}} + \mu \mathcal{O}_{Lm_L}^{\text{mag}}) \right| i \right\rangle \quad (41)$$

$$\xrightarrow{\text{el. only}} -\sum_{LM} i^L \hat{L} \sqrt{2\pi} \left\langle f \left| \left( \frac{1}{ck} \int d\mathbf{x} \mathbf{j}(\mathbf{x}) \cdot \nabla_x \times \mathbf{L} [j_L(kx) Y_{LM}(\Omega_x)] \right) \right| i \right\rangle \quad (42)$$

$$\xrightarrow{k \rightarrow 0} -\sum_{LM} \frac{i^{L+1} \hat{L} \sqrt{2\pi}}{k} \cdot \frac{L+1}{L} \left\langle f \left| \left( \int d\mathbf{x} \mathbf{j}(\mathbf{x}) \cdot \nabla_x [j_L(kx) Y_{LM}(\Omega_x)] \right) \right| i \right\rangle \quad (43)$$

$$= \sum_{LM} i^L \cdot \frac{\hat{L} \sqrt{2\pi}}{\hbar k} \cdot \frac{L+1}{L} \left\langle f \left| \int d\mathbf{x} [\rho(\mathbf{x}), \hat{H}_{\text{nuclear}}] j_L(kx) Y_{LM}(\Omega_x) \right| i \right\rangle \quad (44)$$

$$\stackrel{L=1}{\stackrel{\rho=\rho^{(1)}}{=}} \frac{2}{\hbar k} \left\langle f \left| \sum_i^A q(i) [j_1(kr(i)) Y_{1M}(\Omega_{\mathbf{r}(i)}), \hat{H}_{\text{nuclear}}] \right| i \right\rangle \quad (45)$$

with

$$\mathbf{L} = -i\hbar(\mathbf{x} \times \nabla_x) \quad (46)$$

$$\rho^{(1)}(\mathbf{x}) = \sum_i^A \underbrace{\frac{e}{2}(1 + \tau_z(i))}_{:=q(i)} \delta^{(3)}(\mathbf{x} - \mathbf{r}_i) \quad (47)$$

$$\lim_{x \rightarrow 0} j_l(x) = \frac{x^l}{(2l+1)!!} \quad (48)$$

<sup>43</sup> We abstain

c. *The non-trivial matrix element (which serves **2-body** currents, too)*

$$\left\langle m; l_l m_{l_l} \left| \Phi_{Lm_L}(\boldsymbol{\rho}_\nu) e^{-\beta \mathbf{r}_{ij}} \prod_N^{N_{\text{op}}} \mathcal{Y}_{L_N M_N}(\mathbf{r}_{ij}) \right| l_r m_{l_r}; n \right\rangle \quad (49)$$

<sup>②</sup>rank-L spherical  $\mathbf{L}^2$  tensor

<sup>④</sup>linear combination of spherical  $\mathbf{L}^2$  rank-L tensors, hence, itself a rank-L spherical  $\mathbf{L}^2$  tensor and **not** rank-J spherical  $\mathbf{L}^2$ .

### 44 III. OBTAINING A CROSS SECTION

45 If one is interested in a quantification of the reaction of a nucleus being irradiated with an electromagnetic  
 46 wave, the following formulae might help.

For the total cross section for the reaction of a system initially in state  $\alpha$  induced by a perturbation which transforms  $\alpha$  into a set of final states (labeled  $\alpha'$ ) Taylor (*cf.* [2] Eq.(17.17)) writes

$$\begin{aligned}\sigma(\star \leftarrow \alpha) &= \sum_{\alpha'} \sigma(\alpha' \leftarrow \alpha) \\ &= (2\pi)^4 \frac{m}{k} \sum_{\alpha'} \int d\mathbf{k}' \delta(E' - E) |t(\mathbf{k}', \alpha' \leftarrow \mathbf{k}, \alpha)|^2 \quad .\end{aligned}\tag{50}$$

The perturbation is implicit in the transition matrix  $t$ . For an electromagnetic current,

(51)

#### IV. NOTES ON THE RRGIM IMPLEMENTATION

##### The expansion of the 3-helium ground state

We approximate the antisymmetric nuclear three-body state with the expansion

$$\begin{aligned} \langle \boldsymbol{\rho}_1, \boldsymbol{\rho}_2 \mid {}^3\text{He} \rangle &= \sum_i c_i e^{-\gamma_i \boldsymbol{\rho}_1^2} e^{-\delta_i \boldsymbol{\rho}_2^2} \cdot \left[ [\mathcal{Y}_{l_{1,i}}(\boldsymbol{\rho}_1) \otimes \mathcal{Y}_{l_{2,i}}(\boldsymbol{\rho}_2)]^{L_i} \otimes [(\xi_1 \otimes \xi_2)^{\mathcal{A}_i} \otimes \xi_3]^{S_i} \right]^J \\ &\equiv \sum_i c_i \phi_i(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2) . \end{aligned} \quad (52)$$

A single basis vector is parametrized by two width parameters  $\gamma$  and  $\delta$ , and a (spin) angular-momentum coupling scheme which specifies two angular-momentum quanta  $l_{1,2}$  (one for each Jacobi coordinate  $\boldsymbol{\rho}_{1,2}$ ), a total orbital angular momentum  $L$ , an intermediate spin coupling  $\mathcal{A}$  and the total spin  $S$ .

In practise, we proceed as follows:

1. Fix an orbital-angular-momentum cutoff  $l_{\max}$  and add **all** spin- and orbital coupling schemes to the basis with  $l_{1,2} \leq l_{\max}$  and intermediate/total angular momenta which contribute to a total  $J$  and parity.

The structure  $\left[ [\mathcal{Y}_1(\boldsymbol{\rho}_1) \otimes \mathcal{Y}_1(\boldsymbol{\rho}_2)]^2 \otimes [(\xi_1 \otimes \xi_2)^1 \otimes \xi_3]^{3/2} \right]^{1/2^+}$ , for example, would be included if  $l_{\max} = 2$  and combines two negative-parity solid harmonics to form a of positive parity.

2. For each of the above blocks, two sets of width parameters are chosen. At present, this means selecting upper and lower bounds  $\gamma/\delta_{\min, \max}$  of geometric grids with a fixed number of nodes  $n$ .

For a particular coupling block, one uses  $\gamma \in \{\gamma_{\min}, \gamma_{\max}\}_{\text{geom}}^{n(l_{1,2,i}, L_i, \mathcal{A}_i, S_i)} \equiv w_\gamma$  and  $\delta \in \{\delta_{\min}, \delta_{\max}\}_{\text{geom}}^{m(l_{1,2,i}, L_i, \mathcal{A}_i, S_i)} \equiv w_\delta$ . Hence, for each coupling block there are  $m \cdot n$  (“in principle”) independent Gaussian prefactors. To select those combinations which form a numerically stable and yet complete-for-its-purpose set is an unsolved problem, if the state should be fed into a LIT calculation.



**initial basis** – *the first generation of parents* :

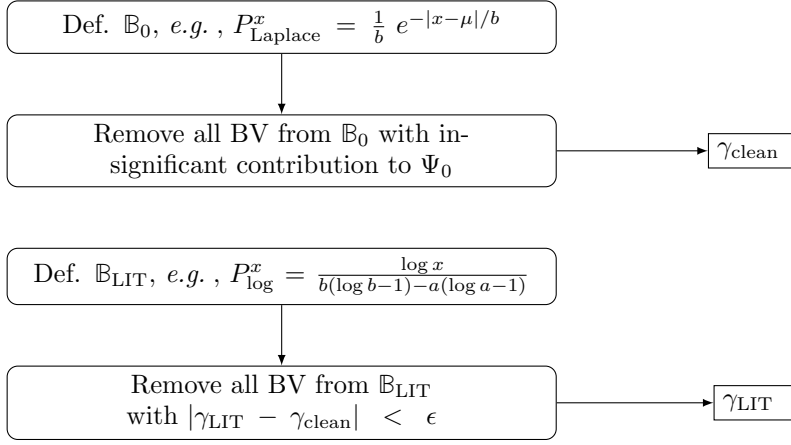
A single basis vector is parametrized by a particular orbital- and (iso)spin angular-momentum coupling scheme,  $\mathbf{cfg}_j := \{l_{1,2}^{(j)}, L^{(j)}, \mathcal{J}^{(j)}, S^{(j)}, \mathcal{J}^{(j)}, T^{(j)}\}$ , **and** a pair of width parameters,  $\mathbf{bv}_i := \{\gamma^{(i)}, \delta^{(i)}\}$ .

We obtain an initial set of vectors by defining **upper** and **lower** bounds within which logarithmically spaced values are selected **for each** **cfg**. As

$$\langle \mathbf{cfg}_n \mathbf{bv}_i \mid \mathbf{cfg}_m \mathbf{bv}_i \rangle \propto \delta_{mn} \quad ,$$

*i.e.* , choosing a basis which contains elements which differ solely in their discrete quantum numbers but have **identical** widths, appears not to introduce linearly dependent vectors, the (anti)symmetrization of the basis,

$$\mathbb{1} := \left\langle \mathbf{cfg}_n \mathbf{bv}_i \mid \hat{\mathcal{A}} \mid \mathbf{cfg}_m \mathbf{bv}_j \right\rangle \quad ,$$



68

69 **luise.f** → **qual.f**

70  $P_{dc}$  and width-independent quantities of  $\Gamma_{l_1 m_1, \dots, l_z m_z}$  with  $z = n_{c_l} - 1 + n_{c_r} - 1 + n_{wv}$ .

71 **obem.f** → **qual.f**

72 **qual.f** → **enemb.f**

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73 WRITE(NBAND1) NZF, MUL, (LREG(K), K=1, NZOPER), I, (NZRHO(K), K=1, NZF)
74
75 WRITE(NBAND1) N3, MMASSE(1, N1, K), MMASSE(2, N1, K), MLAD(1, N1, K),
76 1 MLAD(2, N1, K), MSS(1, N1, K), MSS(2, N1, K), MS(N1, K),
77 2 (LZWERT(L, N2, K), L=1, 5), (RPAR(L, K), L=1, N3), KP(MC1, N4, K)
78
79 WRITE(NBAND1) NTE, NC, ND, ITV2
80
81 WRITE(NBAND1) ((IND(MM, NN), NN=1, JRHO), MM=1, IRHO)
82
83 WRITE(NBAND1) NUML, NUMR, IK1H, JK1H, LL1,
84 * (F(K, L), (J-1, DM(K, L, J), J=1, LL1), L=1, JK1),
85 * K=1, IK1)

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