a. The "LIT equation"

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

with

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

b. The variational basis

$$\Psi_{\rm LIT}^{J^{\pi}m_j} = \sum_n u_n \ \phi_n^{J^{\pi}m_j} \ . \tag{3}$$

with

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

c. The matrix form of the "LIT equation"

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

with

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

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

(8)

(11)

d. The matrix element

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

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

$$(10)$$

$$\underbrace{\hat{J}_{r}\hat{J}_{l}\hat{L}\left\{\begin{array}{ccc} l_{l}^{m} & l_{r}^{n} & p \\ S_{l}^{m} & S_{r}^{n} & q \\ J_{l} & J_{r} & L \end{array}\right\}}_{\text{enemb:ecce}} \underbrace{\sum_{\mathbf{d}c} \sum_{\mathfrak{p} \in \mathbf{d}c} \underbrace{\left\langle m; l_{l}^{m} \mid \mid \mathcal{O}_{p}^{o} \mid \mid \mathcal{A}_{\mathrm{d}c}l_{r}^{n}; n \right.}_{\text{luise}} \cdot \underbrace{\left\langle m; S_{l}^{m} \mid \mid \mathcal{O}_{q}^{s} \mid \mid \mathcal{A}_{\mathfrak{p}}S_{r}^{n}; n \right.}_{\text{obem}}}$$

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

$$\cdot \sum_{\mathrm{dc}} \sum_{\mathrm{p} \in \mathrm{dc}} \left\langle m; l_l^m \mid \right| \mathcal{O}_p^o \mid \mid \mathcal{A}_{\mathrm{dc}} l_r^n; n \rangle \cdot \left\langle m; S_l^m \mid \right| \mathcal{O}_q^s \mid \mid \mathcal{A}_{\mathfrak{p}} S_r^n; n \rangle$$

$$\tag{13}$$

with

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

$$\mathcal{A} = \sum_{\mathfrak{p} \in \mathcal{S}_{A-1}} (-1)^{\operatorname{sgn}(\mathfrak{p})} \hat{\mathfrak{p}} = \bigoplus_{\mathrm{dc}}$$
 (15)

- 1 e. The calculation
 - (i) Solve

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

with ansatz

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

- If \hat{H}_{nuclear} is a spherical rank-0 operator a condition which most practical nuclear potentials satisfy $\Psi^{J_0^{\pi_0}} \neq f(m_{j_0})$. We obtain $\Psi^{J_0J_0}$, in practice.
 - (ii) Calculate

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

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

$$S_{rs,m_L}^{Jm_jJ_0} := \left\langle \phi_r^{J^{\pi}m_j} \mid \hat{\mathcal{O}}_{Lm_L} \mid \phi_s^{J_0^{\pi_0}J_0} \right\rangle ,$$

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

$$S_r^{Jm_j} := \sum_{m_L} \langle LJ_0; m_L m_j - m_L | Jm_j \rangle \underbrace{\sum_{n=0}^{N_0} c_n S_{rn,m_L}^{Jm_j J_0}}_{\text{enemb, f OUT}} . \tag{17}$$

- 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

$$\left(\mathbb{H}_{rs} - \mathcal{E}\mathbb{N}_{rs}\right) u_s^{Jm_j} = S_r^{Jm_j} \tag{18}$$

to obtain the LIT state

$$\psi_{J_{i(\text{nitial})/f(\text{inal})};J_{(i)n(\text{termediate})}m_{n}}^{v(\text{ertex}),(\text{mu})L(\text{tipolarity})}(k,\sigma) = \psi_{J_{0};Jm_{j}}^{v,L}(k,\sigma) := \Psi_{\text{LIT}}^{J^{\pi}m_{j}} \left(\underbrace{|\mathbf{k}|,v,L}_{\text{vertex}}; \underbrace{E_{0},J_{0}}_{\text{initial/final-state}}; \mathcal{R}\left[\sigma\right], \mathcal{I}\left[\sigma\right] \right) .$$

$$(19)$$

(v) The inner product

$$\mathcal{L}_{v'L',vL}^{J_f,J_i;J}(k',k,\sigma) = (-1)^{J-J_i+L-L'+v'} N_{J,\sigma} \sum_{m_j} \underbrace{\left\langle \psi_{J_f;Jm_j}^{v',L'}(k',\sigma) \middle| \psi_{J_i;Jm_j}^{v,L}(k,\sigma) \right\rangle}_{=\sum_{r,s} (u_r^{Jm_j})^* u_s^{Jm_j} \mathbb{N}_{rs}}$$
(20)

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

(21)

8 I. FORMULAS AND CONSTANTS

(Wigner) 3-
$$j$$
 symbol:
$$\begin{pmatrix} L & S & J \\ m_l & m_s & -m_j \end{pmatrix} = (-1)^{L-S+m_j} (2J+1)^{-\frac{1}{2}} \langle LS; m_l m_s | J m_j \rangle \quad (22)$$
Matrix for single-axis rotation:
$$\mathcal{D}_{m',m}^{(j)}(0 \ \beta \ 0) \equiv d_{m',m}^{(j)}(\beta)$$

$$= \left[\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!} \right]^{\frac{1}{2}}$$

$$\cdot \sum_{\sigma} \begin{pmatrix} j+m \\ j-m'-\sigma \end{pmatrix} \begin{pmatrix} j-m \\ \sigma \end{pmatrix} (-1)^{j-m'-\sigma}$$

$$\cdot \left(\cos \frac{\beta}{2} \right)^{2\sigma+m+m'} \left(\sin \frac{\beta}{2} \right)^{2j-2\sigma-m-m'} \quad (23)$$

$$(24)$$

a. The Lorentz transformation of a Lorentzian

The strength functions which constitute the Compton amplitudes are themselves composed of scalar functions of an energy parameter. I assume that these functions can be expanded to any desired accuracy in a Lorentzian/2 Cauchy basis as follows:

$$r(e) = \sum_{n} c_n \frac{\theta(e - e_{\text{th}})}{(a_n - e)^2 + b_n^2} := \sum_{n} c_n \theta(e - e_{\text{th}}) f_n .$$
 (25)

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

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

$$L(\sigma) := \int_{-\infty}^{\infty} \frac{r(e)}{(\sigma_r - e)^2 + \sigma_i^2} de = \sum_n c_n \int_{e_{\text{th}}}^{\infty} \frac{f_n(e)}{(\sigma_r - e)^2 + \sigma_i^2} de .$$
 (26)

If basis basis functions[®] which we define through the integral

$$\int_{e_{\text{th}}}^{\infty} \frac{f_n(e)}{(\sigma_r - e)^2 + \sigma_i^2} de = \int_{e_{\text{th}}}^{\infty} \frac{1}{(\sigma_r - e)^2 + \sigma_i^2} \cdot \frac{1}{(a_n - e)^2 + b_n^2} de$$

$$\vdots$$

$$= \left[(\sigma_r - a_n)^2 + (\sigma_i - b_n)^2 \right]^{-1} \cdot \left[(\sigma_r - a_n)^2 + (\sigma_i + b_n)^2 \right]^{-1}$$

$$\cdot \left\{ \sigma_i^{-1} \left((\sigma_r - a_n)^2 + b_n^2 - \sigma_i^2 \right) \left(\frac{\pi}{2} + \tan^{-1} \left(\frac{\sigma_r'}{\sigma_i} \right) \right) + b_n^{-1} \left((\sigma_r - a_n)^2 - b_n^2 + \sigma_i^2 \right) \left(\frac{\pi}{2} + \tan^{-1} \left(\frac{a_n'}{b_n} \right) \right) + (\sigma_r - a_n) \ln \left(\frac{\sigma_r'^2 + \sigma_i^2}{a_n'^2 + b_n^2} \right) \right\}$$

$$:= L_n(\sigma, e_{\text{th}})$$

 $^{\textcircled{1}}x' := x - e_{\operatorname{th}}$

$\alpha = \frac{e^2}{4\pi}$	dimensionless	$\frac{1}{137.03604}$	(2	(28)
$\hbar c$		$197.32858~\mathrm{MeV}\cdot\mathrm{fm}^2$		

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

$$\min_{\mathbf{c}} \left| L(\sigma) - \sum_{n} c_n L_n(\sigma, e_{\text{th}}) \right| := \mathbf{c}^*. \tag{27}$$

The set of optimal parameters c^* represents via Eq.(25) an expansion of the response function in Lorentzians. ²⁰ 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.

22 II. "HOW TO DO AN INTEGRAL"

- 23 a. The multipole operators
 - convection current[®]

$$\boldsymbol{j}_{o}(\boldsymbol{x}) = \frac{e}{2m} \sum_{i}^{A} \frac{1}{2} \left(1 + \tau_{z}(i) \right) \left\{ \boldsymbol{p}(i) , \delta^{(3)}(\boldsymbol{x} - \boldsymbol{r}(i)) \right\}$$
(29a)

(electric)
$$\mathcal{O}_{Lm_L}^{o^{\text{el}}} = \frac{e\hbar}{mc} \hat{L}^{-1} \sum_{i}^{A} g_l(i) \left[\sqrt{L} \Delta_{LM}^{L+1}(\boldsymbol{r}(i)) - \sqrt{L+1} \Delta_{LM}^{L-1}(\boldsymbol{r}(i)) \right]$$
 (29b)

(magnetic)
$$\mathcal{O}_{Lm_L}^{o^{\text{mag}}} = i \frac{e\hbar}{mc} \sum_{i}^{A} g_l(i) \Delta_{LM}^L(\boldsymbol{r}(i))$$
 (29c)

• spin current

$$\boldsymbol{j}_{s}(\boldsymbol{x}) = \frac{e\hbar}{2m} \sum_{i}^{A} \frac{1}{2} \left(g_{s_{p}} \left(1 + \tau_{z}(i) \right) + g_{s_{n}} \left(1 - \tau_{z}(i) \right) \right) \boldsymbol{\sigma}(i) \times \boldsymbol{\nabla}(i) \delta^{(3)}(\boldsymbol{x} - \boldsymbol{r}(i))$$
(30a)

(electric)
$$\mathcal{O}_{Lm_L}^{s^{\text{el}}} = -\frac{e\hbar |\mathbf{k}|}{2mc} \sum_{i}^{A} g_s(i) \sum_{M\nu} \langle L1; M\nu | Lm_L \rangle \cdot \boldsymbol{\sigma}_{\nu}(i) \Phi_{LM}(\mathbf{r}(i))$$
 (30b)

(magnetic)
$$\mathcal{O}_{Lm_L}^{s^{\text{mag}}} = i \frac{e\hbar |\mathbf{k}|}{2mc} \hat{L}^{-1} \sum_{i}^{A} g_s(i) \sum_{M,\nu} \left[\sqrt{L} \langle L+11; M\nu | Lm_L \rangle \boldsymbol{\sigma}_{\nu}(i) \Phi_{L+1M}(\boldsymbol{r}(i)) \right]$$
 (30c)

$$-\sqrt{L+1} \langle L-11; M\nu \mid Lm_L \rangle \boldsymbol{\sigma}_{\nu}(i) \Phi_{L-1M}(\boldsymbol{r}(i))$$
(30d)

^①Indices referring to particles are put in brackets.

with

$$\Phi_{Lm_L}(\mathbf{r}) = j_L(kr) Y_{Lm_L}(\Omega_r) \tag{31}$$

$$\Delta_{Lm_L}^J(\mathbf{r}) = \sum_{M,\nu} \langle L1; M\nu \mid Jm_L \rangle \Phi_{Lm_L}(\mathbf{r}) \mathbf{p}_{\nu} . \tag{32}$$

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b. Siegert form

$$\left\langle f \mid \left(\frac{1}{ck} \int d\mathbf{x} \ \mathbf{j}(\mathbf{x}) \cdot \nabla_x \times \mathbf{L} \left[j_L(kx) Y_{LM}(\Omega_x) \right] \right) \mid i \right\rangle$$
 (33)

$$\stackrel{k \to 0}{=} \frac{i}{k} \frac{L+1}{L} \left\langle f \mid \left(\int d\mathbf{x} \ \mathbf{j}(\mathbf{x}) \cdot \nabla_x \left[j_L(kx) Y_{LM}(\Omega_x) \right] \right) \mid i \right\rangle$$
(34)

$$= \frac{1}{\hbar k} \frac{L+1}{L} \left\langle f \mid \int d\boldsymbol{x} \left[\rho(\boldsymbol{x}), \, \hat{H}_{\text{nuclear}} \right] \, j_L(kx) Y_{LM}(\Omega_x) \mid i \right\rangle$$
 (35)

$$\stackrel{L=1}{=} \stackrel{\&}{=} \stackrel{\rho=\rho^{(1)}}{=} \frac{2}{\hbar k} \left\langle f \left| \sum_{i}^{A} q(i) \left[j_{1}(kr(i)) Y_{1M}(\Omega_{r(i)}), \hat{H}_{\text{nuclear}} \right] \right| i \right\rangle$$
(36)

with

$$\boldsymbol{L} = -i\hbar \left(\boldsymbol{x} \times \boldsymbol{\nabla}_{x} \right) \tag{37}$$

$$\rho^{(1)}(\mathbf{x}) = \sum_{i}^{A} \underbrace{\frac{e}{2}(1 + \tau_{z}(i))}_{:=q(i)} \delta^{(3)}(\mathbf{x} - \mathbf{r}_{i})$$
(38)

$$\lim_{x \to 0} j_l(x) = \frac{x^l}{(2l+1)!!} \tag{39}$$

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

$$\left\langle m; l_l m_{l_l} \middle| \Phi_{Lm_L}(\boldsymbol{\rho_{\nu}}) e^{-\beta \boldsymbol{r}_{ij}} \prod_{N}^{N_{\text{op}}} \mathcal{Y}_{L_N M_N}(\boldsymbol{r}_{ij}) \middle| l_r m_{l_r}; n \right\rangle$$
(40)

 $^{@}\mathrm{rank\text{-}L}$ spherical \boldsymbol{L}^{2} tensor

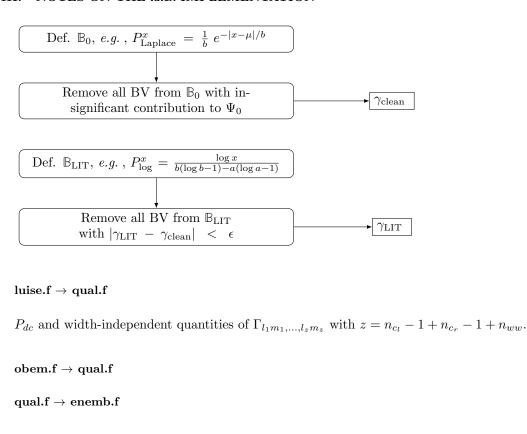
[®] linear combination of spherical L^2 rank-L tensors, hence, itself a rank-L spherical L^2 tensor and not rank-J spherical L^2 .

25 III. NOTES ON THE RRGM IMPLEMENTATION

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37 38

39 40



WRITE(NBAND1) ((IND(MM,NN), NN=1, JRHO), MM=1, IRHO)

2 (LZWERT(L,N2,K),L=1,5),(RPAR(L,K),L=1,N3),KP(MC1,N4,K)

1 MLAD(2,N1,K),MSS(1,N1,K),MSS(2,N1,K),MS(N1,K),

WRITE (NBAND1) NTE, NC, ND, ITV2

WRITE(NBAND1) NZF,MUL,(LREG(K),K=1,NZOPER),I,(NZRHO(K),K=1,NZF)

WRITE (NBAND1) N3, MMASSE (1, N1, K), MMASSE (2, N1, K), MLAD (1, N1, K),