

a. The “LIT equation”

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

with

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

b. The variational basis

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

with

$$\phi_n^{J^\pi m_j} = [\xi_{S_n} \otimes \mathcal{Y}_{l_n}(\boldsymbol{\rho})]^{Jm_j} e^{-\gamma_n \boldsymbol{\rho}^2} \quad (\text{i.e. , LS coupling}) ; \quad (4)$$

c. The matrix form of the “LIT equation”

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

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

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

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

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

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

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

with

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

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

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

e. The calculation

(i) Solve

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

with ansatz

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

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 $\Psi^{J_0 J_0}$, 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

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

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

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

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

(iv) Solve the (complex) linear matrix equation

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

to obtain the LIT state

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

(v) The inner product

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

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

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:

$$\begin{aligned} \mathcal{D}_{m',m}^{(j)}(0 \ \beta \ 0) &\equiv d_{m',m}^{(j)}(\beta) \\ &= \left[\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!} \right]^{\frac{1}{2}} \\ &\quad \cdot \sum_{\sigma} \begin{pmatrix} j+m \\ j-m'-\sigma \end{pmatrix} \begin{pmatrix} j-m \\ \sigma \end{pmatrix} (-1)^{j-m'-\sigma} \\ &\quad \cdot \left(\cos \frac{\beta}{2} \right)^{2\sigma+m+m'} \left(\sin \frac{\beta}{2} \right)^{2j-2\sigma-m-m'} \end{aligned} \quad (23)$$

9 II. CODE

luise.f \rightarrow qual.f

P_{dc} and width-independent quantities of $\Gamma_{l_1 m_1, \dots, l_z m_z}$ with $z = n_{cl} - 1 + n_{cr} - 1 + n_{ww}$.

obem.f \rightarrow qual.f

qual.f \rightarrow enemb.f

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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),
1 MLAD(2, N1, K), MSS(1, N1, K), MSS(2, N1, K), MS(N1, K),
2 (LZWERT(L, N2, K), L=1, 5), (RPAR(L, K), L=1, N3), KP(MC1, N4, K)
WRITE(NBAND1) NTE, NC, ND, ITV2
WRITE(NBAND1) ((IND(MM, NN), NN=1, JRHO), MM=1, IRHO)
WRITE(NBAND1) NUML, NUMR, IK1H, JK1H, LL1,
* ((F(K, L), (J-1, DM(K, L, J), J=1, LL1), L=1, JK1),
* K=1, IK1)

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27 III. “HOW TO DO AN INTEGRAL”

a. *The multipole operators*

- convection current^①

$$\mathbf{j}_o(\mathbf{x}) = \frac{e}{2m} \sum_i \frac{1}{2} (1 + \tau_z(i)) \left\{ \mathbf{p}(i), \delta^{(3)}(\mathbf{x} - \mathbf{r}(i)) \right\} \quad (24a)$$

$$\text{(electric)} \mathcal{O}_{Lm_L}^{\text{el}} = \frac{e\hbar}{mc} \hat{L}^{-1} \sum_i g_l(i) \left[\sqrt{L} \Delta_{LM}^{L+1}(\mathbf{r}(i)) - \sqrt{L+1} \Delta_{LM}^{L-1}(\mathbf{r}(i)) \right] \quad (24b)$$

$$\text{(magnetic)} \mathcal{O}_{Lm_L}^{\text{mag}} = i \frac{e\hbar}{mc} \sum_i g_l(i) \Delta_{LM}^L(\mathbf{r}(i)) \quad (24c)$$

- spin current

$$\mathbf{j}_s(\mathbf{x}) = \frac{e\hbar}{2m} \sum_i \frac{1}{2} (g_{s_p} (1 + \tau_z(i)) + g_{s_n} (1 - \tau_z(i))) \boldsymbol{\sigma}(i) \times \boldsymbol{\nabla}(i) \delta^{(3)}(\mathbf{x} - \mathbf{r}(i)) \quad (25a)$$

$$\text{(electric)} \mathcal{O}_{Lm_L}^{\text{el}} = - \frac{e\hbar |\mathbf{k}|}{2mc} \sum_i g_s(i) \sum_{M,\nu} \langle L1; M\nu | Lm_L \rangle \cdot \boldsymbol{\sigma}_\nu(i) \Phi_{LM}(\mathbf{r}(i)) \quad (25b)$$

$$\text{(magnetic)} \mathcal{O}_{Lm_L}^{\text{mag}} = i \frac{e\hbar |\mathbf{k}|}{2mc} \hat{L}^{-1} \sum_i g_s(i) \sum_{M,\nu} \left[\sqrt{L} \langle L+11; M\nu | Lm_L \rangle \boldsymbol{\sigma}_\nu(i) \Phi_{L+1M}(\mathbf{r}(i)) \right. \quad (25c)$$

$$\left. - \sqrt{L+1} \langle L-11; M\nu | Lm_L \rangle \boldsymbol{\sigma}_\nu(i) \Phi_{L-1M}(\mathbf{r}(i)) \right] \quad (25d)$$

with

$$\Phi_{Lm_L}(\mathbf{r}) = j_L(kr) Y_{Lm_L}(\Omega_r) \quad \text{②} \quad (26)$$

$$\Delta_{Lm_L}^J(\mathbf{r}) = \sum_{M,\nu} \langle L1; M\nu | Jm_L \rangle \Phi_{Lm_L}(\mathbf{r}) \mathbf{p}_\nu \quad \text{③} \quad (27)$$

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b. Siegert form

$$\left\langle f \left| \left(\frac{1}{ck} \int d\mathbf{x} \mathbf{j}(\mathbf{x}) \cdot \boldsymbol{\nabla}_x \times \mathbf{L} [j_L(kx) Y_{LM}(\Omega_x)] \right) \right| i \right\rangle \quad (28)$$

$$\stackrel{k \rightarrow 0}{=} \frac{i}{k} \frac{L+1}{L} \left\langle f \left| \left(\int d\mathbf{x} \mathbf{j}(\mathbf{x}) \cdot \boldsymbol{\nabla}_x [j_L(kx) Y_{LM}(\Omega_x)] \right) \right| i \right\rangle \quad (29)$$

$$= \frac{1}{\hbar k} \frac{L+1}{L} \left\langle f \left| \int d\mathbf{x} \left[\rho(\mathbf{x}), \hat{H}_{\text{nuclear}} \right] j_L(kx) Y_{LM}(\Omega_x) \right| i \right\rangle \quad (30)$$

$$\stackrel{L=1}{=} \stackrel{\& \rho=\rho^{(1)}}{=} \frac{2}{\hbar k} \left\langle f \left| \sum_i q(i) \left[j_1(kr(i)) Y_{1M}(\Omega_{\mathbf{r}(i)}), \hat{H}_{\text{nuclear}} \right] \right| i \right\rangle \quad (31)$$

^①Indices referring to particles are put in brackets.

^③rank-L spherical \mathbf{L}^2 tensor

^⑤linear 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 .

with

$$\mathbf{L} = -i\hbar(\mathbf{x} \times \nabla_{\mathbf{x}}) \quad (32)$$

$$\rho^{(1)}(\mathbf{x}) = \sum_i^A \underbrace{\frac{e}{2}(1 + \tau_z(i))}_{:=q(i)} \delta^{(3)}(\mathbf{x} - \mathbf{r}_i) \quad (33)$$

$$\lim_{x \rightarrow 0} j_l(x) = \frac{x^l}{(2l+1)!!} \quad (34)$$

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

$$\left\langle m; l_l m_{l_l} \left| \Phi_{L m_L}(\boldsymbol{\rho}_{\nu}) e^{-\beta \mathbf{r}_{ij}} \prod_N^{N_{\text{op}}} \mathcal{Y}_{L_N M_N}(\mathbf{r}_{ij}) \right| l_r m_{l_r}; n \right\rangle \quad (35)$$