a. The "LIT equation"

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

with

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

b. The variational basis

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

with

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

c. The matrix form of the "LIT equation"

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

with

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

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

$$\tag{8}$$

d. The matrix element

$$\phi_m^{J^\pi m_j}\ \hat{\mathcal{O}}_{Lm_L}\ \phi_n^{J_0^{\pi_0}m_{j_0}} := \langle\, m; l_lS_lJ_lm_{j_l}\ |\ \mathcal{A}\ \mathcal{O}_{Lm_L}\ |\ l_rS_rJ_rm_{j_r};n\,\rangle \tag{9}$$

$$= \underbrace{(-1)^{L-J_r+J_l}\frac{\langle\, LJ_r\,;\,m_Lm_{j_r}\,|\ \ J_lm_{j_l}\,\rangle}{\hat{J}_l}}_{\texttt{enemb:600ff}}\underbrace{\langle\, m; l_lS_lJ_l\,||\ \mathcal{A}\ \mathcal{O}_L\ ||\,l_rS_rJ_r;n\,\rangle}_{} \tag{10}$$

$$\underbrace{\hat{J}_r\hat{J}_l\hat{L}\begin{Bmatrix} l_l^m & l_r^n & p \\ S_l^m & S_r^n & q \\ J_l & J_r & L\end{Bmatrix}}_{\texttt{enemb:ecce}}\sum_{\mathrm{dc}}\sum_{\mathfrak{p}\in\mathrm{dc}}\underbrace{\langle\, m; l_l^m\ ||\ \mathcal{O}_p^o\ ||\,\mathcal{A}_{\mathrm{dc}}l_r^n;n\,\rangle}_{\texttt{luise}}\cdot\underbrace{\langle\, m; S_l^m\ ||\ \mathcal{O}_q^s\ ||\,\mathcal{A}_{\mathfrak{p}}S_r^n;n\,\rangle}_{\texttt{obem}} \tag{11}$$

$$= \hat{J}_r\hat{L}\,\langle\, J_rL\,;\,m_{j_r}m_L\,|\ \ J_lm_{j_l}\,\rangle\cdot\begin{Bmatrix} l_l^m & l_r^n & p \\ S_l^m & S_r^n & q \\ J_l & J_r & L\end{Bmatrix} \tag{12}$$

$$\cdot\sum_{\mathrm{dc}}\sum_{\mathfrak{p}\in\mathrm{dc}}\langle\, m; l_l^m\ ||\ \mathcal{O}_p^o\ ||\,\mathcal{A}_{\mathrm{dc}}l_r^n;n\,\rangle\cdot\langle\, m; S_l^m\ ||\ \mathcal{O}_q^s\ ||\,\mathcal{A}_{\mathfrak{p}}S_r^n;n\,\rangle \tag{13}$$

with

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

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

$$\mathrm{dc}\ \ :\ \ \text{double co-set} \tag{16}$$

e. The calculation

(i) Solve

$$\hat{H}_{\text{nuclear}}\ \Psi^{J_0^{\pi 0}} = E_0\ \Psi^{J_0^{\pi 0}}$$

with the ansatz

$$\Psi^{J_0^{\pi 0}} = \sum_n c_n\ \phi_n^{J_0^{\pi 0}} \quad .$$

If $\hat{H}_{\text{nuclear}}$ 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

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

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

$$S^{Jm_jJ_0}_{rs,m_L} := \left\langle\ \phi_r^{J^\pi m_j}\ \middle|\ \hat{\mathcal{O}}_{Lm_L}\ \middle|\ \phi_s^{J_0^{\pi 0}J_0}\ \right\rangle \quad ,$$

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

$$S_r^{Jm_j} := \sum_{m_L}\ \langle\ LJ_0\,;\, m_L m_j{-}m_L\ |\ \ Jm_j\ \rangle\ \underbrace{\sum_n^{N_0}\ c_n\ S^{Jm_jJ_0}_{rn,m_L}}_{\textbf{enemb.f OUT}} \quad . \tag{17}$$

Ecce, $\Psi^{J_0^{\pi 0}} \neq f(m_{j_0})$ does not allow for an elimination of m_j from this equation!

(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

$$\psi^{v(\text{ertex}),(\text{mu})L(\text{tipolarity})}_{J_{i(\text{nitial})/f(\text{inal})};J_{(\text{i})n(\text{termediate})}m_n}(k,\sigma) = \psi^{v,L}_{J_0;Jm_j}(k,\sigma) := \Psi^{J^\pi m_j}_{\text{LIT}}\Big(\ \underbrace{|\boldsymbol{k}|\,,v,L}_{\substack{\text{vertex}\\ \text{quantum numbers}}}\ \ ;\ \ \underbrace{E_0,J_0}_{\substack{\text{initial/final-state}\\ \text{quantum numbers}}}\ \ ;\mathcal{R}\,[\sigma]\,,\mathcal{I}\,[\sigma]\,\Big) \quad . \tag{19}$$

(v) The inner product

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

$$= \int_{e_{\text{th}}}^{\infty} \frac{\mathcal{F}^{J_f,J_i;J}_{v'L',vL}(k',k,E)}{(E-\sigma)(E-\sigma^*)}\ dE \tag{21}$$

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

$$\tag{22}$$

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

At this stage, the problem is to recover $\mathcal{F}$, given $\mathcal{L}$ by inverting the integral transformation Eq. (21). The *discrete essence* of that can be written as

$$\boldsymbol{L}_s = \sum_e A_{se} \boldsymbol{F}^e = \sum_n c_n \sum_e A_{se} f_n^e \quad . \tag{23}$$

If the energy sum/integral can be evaluated efficiently for a set of basis vectors f_n which is suitable for a proper representation of the vector $\boldsymbol{L}$, it remains to solve a linear optimization problem. This is detailed below from Eq. (28) onwards.

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

$$\mathcal{F}^{J_f,J_i;J}_{v'L',vL}(k',k,E) = \underbrace{N_{J,E}}_{\#J,E-\text{states}} \langle\, J_f\ E_f \,||\, M^{\nu',L'}(k') \,||\, J\ E \,\rangle \,\langle\, J\ E \,||\, M^{\nu,L}(k) \,||\, J_i\ E_i \,\rangle \quad , \tag{24}$$

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

The second, related idea for choosing a Lorentz basis is the ability to calculate the integral transform with a Lorentz kernel analytically (viz. Eq. (30)).

I. FORMULAS AND CONSTANTS

$$\text{(Wigner) 3-}j\text{ symbol:} \qquad \begin{pmatrix} L & S & J \\ m_l & m_s & -m_j \end{pmatrix} = (-1)^{L-S+m_j} \; (2J+1)^{-\frac{1}{2}} \; \langle \, LS\,;\, m_l m_s \,|\; J m_j \, \rangle \tag{25}$$

$$\begin{aligned} \text{Matrix for single-axis rotation:} \qquad \mathcal{D}^{(j)}_{m',m}(0\;\beta\;0) &\equiv d^{(j)}_{m',m}(\beta) \\ &= \left[\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!}\right]^{\frac{1}{2}} \\ &\quad \cdot \sum_{\sigma} \begin{pmatrix} j+m \\ j-m'-\sigma \end{pmatrix} \begin{pmatrix} j-m \\ \sigma \end{pmatrix} (-1)^{j-m'-\sigma} \\ &\quad \cdot \left(\cos\frac{\beta}{2}\right)^{2\sigma+m+m'} \left(\sin\frac{\beta}{2}\right)^{2j-2\sigma-m-m'} \end{aligned} \tag{26}$$

$$\tag{27}$$

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/-Cauchy basis as follows:

$$r(e) = \sum_n c_n \frac{\theta(e-e_{\text{th}})}{(a_n-e)^2+b_n^2} := \sum_n c_n \theta(e-e_{\text{th}}) f_n \;. \tag{28}$$

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

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

$$L(\sigma) := \int\limits_{-\infty}^{\infty} \frac{r(e)}{(\sigma_r-e)^2+\sigma_i^2}\; de = \sum_n c_n \int\limits_{e_{\text{th}}}^{\infty} \frac{f_n(e)}{(\sigma_r-e)^2+\sigma_i^2}\; de \;. \tag{29}$$

If basis basis functions[1] which we define through the integral

$$\begin{aligned} \int_{e_{\text{th}}}^{\infty} \frac{f_n(e)}{(\sigma_r-e)^2+\sigma_i^2}\; de \;&=\; \int_{e_{\text{th}}}^{\infty} \frac{1}{(\sigma_r-e)^2+\sigma_i^2} \cdot \frac{1}{(a_n-e)^2+b_n^2}\; de \\ &\;\;\vdots \\ &=\; \left[(\sigma_r-a_n)^2+(\sigma_i-b_n)^2\right]^{-1} \cdot \left[(\sigma_r-a_n)^2+(\sigma_i+b_n)^2\right]^{-1} \\ &\quad \cdot \Bigg\{ \sigma_i^{-1}\left((\sigma_r-a_n)^2+b_n^2-\sigma_i^2\right)\left(\frac{\pi}{2}+\tan^{-1}\left(\frac{\sigma_r'}{\sigma_i}\right)\right) \\ &\quad + b_n^{-1}\left((\sigma_r-a_n)^2-b_n^2+\sigma_i^2\right)\left(\frac{\pi}{2}+\tan^{-1}\left(\frac{a_n'}{b_n}\right)\right) \\ &\quad + (\sigma_r-a_n)\;\ln\left(\frac{{\sigma_r'}^2+\sigma_i^2}{{a_n'}^2+b_n^2}\right) \Bigg\} \\ &:= L_n(\sigma, e_{\text{th}}) \end{aligned} \tag{30}$$

---

[1] $x' := x - e_{\text{th}}$

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

(32)

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

$$\min_{\boldsymbol{c}} \left| L(\sigma) - \sum_n c_n L_n(\sigma, e_{\text{th}}) \right| := \boldsymbol{c}^*. \tag{31}$$

The set of optimal parameters $\boldsymbol{c}^*$ represents via Eq. (28) 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[1]

$$\boldsymbol{j}_o(\boldsymbol{x}) = \frac{e}{2m} \sum_i^A \frac{1}{2} \left(1 + \tau_z(i)\right) \left\{ \boldsymbol{p}(i) \ , \ \delta^{(3)}(\boldsymbol{x} - \boldsymbol{r}(i)) \right\} \tag{33a}$$

$$\textbf{(electric)}\ \mathcal{O}^{o^{\text{el}}}_{Lm_L} = \frac{e\hbar}{mc} \hat{L}^{-1} \sum_i^A g_l(i) \left[\sqrt{L} \Delta^{L+1}_{LM}(\boldsymbol{r}(i)) - \sqrt{L+1} \Delta^{L-1}_{LM}(\boldsymbol{r}(i)) \right] \tag{33b}$$

$$\textbf{(magnetic)}\ \mathcal{O}^{o^{\text{mag}}}_{Lm_L} = i \frac{e\hbar}{mc} \sum_i^A g_l(i) \Delta^L_{LM}(\boldsymbol{r}(i)) \tag{33c}$$

- spin current

$$\boldsymbol{j}_s(\boldsymbol{x}) = \frac{e\hbar}{2m} \sum_i^A \frac{1}{2} \left(g_{s_p} \left(1 + \tau_z(i)\right) + g_{s_n} \left(1 - \tau_z(i)\right) \right) \boldsymbol{\sigma}(i) \times \boldsymbol{\nabla}(i) \delta^{(3)}(\boldsymbol{x} - \boldsymbol{r}(i)) \tag{34a}$$

$$\textbf{(electric)}\ \mathcal{O}^{s^{\text{el}}}_{Lm_L} = - \frac{e\hbar|\boldsymbol{k}|}{2mc} \sum_i^A g_s(i) \sum_{M,\nu} \langle\, L1\,;\, M\nu \,|\ \ Lm_L \,\rangle \cdot \boldsymbol{\sigma}_\nu(i) \Phi_{LM}(\boldsymbol{r}(i)) \tag{34b}$$

$$\textbf{(magnetic)}\ \mathcal{O}^{s^{\text{mag}}}_{Lm_L} = i \frac{e\hbar|\boldsymbol{k}|}{2mc} \hat{L}^{-1} \sum_i^A g_s(i) \sum_{M,\nu} \Big[\sqrt{L}\, \langle\, L+11\,;\, M\nu \,|\ \ Lm_L \,\rangle\, \boldsymbol{\sigma}_\nu(i) \Phi_{L+1M}(\boldsymbol{r}(i)) \tag{34c}$$

$$- \sqrt{L+1}\, \langle\, L-11\,;\, M\nu \,|\ \ Lm_L \,\rangle\, \boldsymbol{\sigma}_\nu(i) \Phi_{L-1M}(\boldsymbol{r}(i)) \Big] \tag{34d}$$

---

[1] Indices referring to particles are put in brackets.

with

$$\Phi_{Lm_L}(\boldsymbol{r}) = j_L(kr)\ Y_{Lm_L}(\Omega_r) \qquad ① \tag{35}$$

$$\Delta^J_{Lm_L}(\boldsymbol{r}) = \sum_{M,\nu} \langle\ L1\ ;\ M\nu \mid\ \ Jm_L\ \rangle\, \Phi_{Lm_L}(\boldsymbol{r})\ \boldsymbol{p}_\nu\ \ . \qquad ② \tag{36}$$

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b. *Siegert form*

$$\left\langle\ f\ \middle|\ \left(\frac{1}{ck}\int d\boldsymbol{x}\ \boldsymbol{j}(\boldsymbol{x})\cdot\boldsymbol{\nabla}_x\times\boldsymbol{L}\left[j_L(kx)Y_{LM}(\Omega_x)\right]\right)\ \middle|\ i\ \right\rangle \tag{37}$$

$$\overset{k\to 0}{=}\ \frac{i}{k}\frac{L+1}{L}\left\langle\ f\ \middle|\ \left(\int d\boldsymbol{x}\ \boldsymbol{j}(\boldsymbol{x})\cdot\boldsymbol{\nabla}_x\left[j_L(kx)Y_{LM}(\Omega_x)\right]\right)\ \middle|\ i\ \right\rangle \tag{38}$$

$$=\frac{1}{\hbar k}\frac{L+1}{L}\left\langle\ f\ \middle|\ \int d\boldsymbol{x}\ \left[\rho(\boldsymbol{x})\,,\,\hat{H}_{\text{nuclear}}\right]\ j_L(kx)Y_{LM}(\Omega_x)\ \middle|\ i\ \right\rangle \tag{39}$$

$$\overset{L=1\ \&\ \rho=\rho^{(1)}}{=}\ \frac{2}{\hbar k}\left\langle\ f\ \middle|\ \sum_i^A\ q(i)\ \left[j_1(kr(i))Y_{1M}(\Omega_{\boldsymbol{r}(i)})\,,\,\hat{H}_{\text{nuclear}}\right]\ \middle|\ i\ \right\rangle \tag{40}$$

with

$$\boldsymbol{L} = -\,i\hbar\,(\boldsymbol{x}\times\boldsymbol{\nabla}_x) \tag{41}$$

$$\rho^{(1)}(\boldsymbol{x}) = \sum_i^A \underbrace{\frac{e}{2}(1+\tau_z(i))}_{:=q(i)}\,\delta^{(3)}(\boldsymbol{x}-\boldsymbol{r}_i) \tag{42}$$

$$\lim_{x\to 0} j_l(x) = \frac{x^l}{(2l+1)!!} \tag{43}$$

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

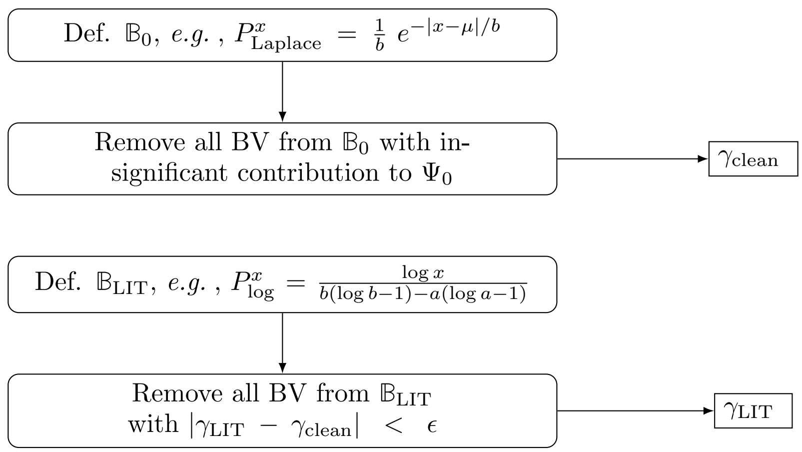
$$\left\langle\ m;l_l m_{l_l}\ \middle|\ \Phi_{Lm_L}(\boldsymbol{\rho_\nu})\ e^{-\beta\boldsymbol{r}_{ij}}\prod_N^{N_{\text{op}}}\mathcal{Y}_{L_N M_N}(\boldsymbol{r}_{ij})\ \middle|\ l_r m_{l_r};n\ \right\rangle \tag{44}$$

---

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

④linear combination of spherical $\boldsymbol{L}^2$ rank-L tensors, hence, itself a rank-L spherical $\boldsymbol{L}^2$ tensor and not rank-J spherical $\boldsymbol{L}^2$.

III. NOTES ON THE RRGM IMPLEMENTATION



luise.f → qual.f

P_{dc} and width-independent quantities of $\Gamma_{l_1m_1,\ldots,l_zm_z}$ with $z = n_{c_l} - 1 + n_{c_r} - 1 + n_{ww}$.

obem.f → qual.f

qual.f → enemb.f

```
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)
```