a. ....

calculation flow

1. `git clone git@github.com:kirschjs/LIT_source.git`
2. `make all` in `./LIT_source/src_nucl/`, `./LIT_source/src_nucl/V18_PAR/`, `./LIT_source/src_nucl/UIX_PAR/`, and `./LIT_source/src_elma_pol/`
3. `cd ./LIT_source/src_python/EugenicistsApproach`
4. `./python3.x NextToNewestGeneration.py`
5. `./python3.x A3_lit_M.py`
6. `mathematica ./LIT_source/src_mathematica/helion_E1_multiBas_crosssection.nb`
7. set `resultsDir` in 3rd cell to the directory specified by the last output of `A3_lit_M.py`

support: `kirscjo@gmail.com` or `skype` to `kirschjs.dc` ;

code repository: `git clone git@github.com:kirschjs/LIT_source.git`

1. optimize bases for final and initial states

calculation flow step (4)

`NextToNewestGeneration.py`

argument	comment
bastypes	see `bridgeA3.py` for the defined structures, *e.g.*, $\left\vert\, {}^3\mathrm{He} \right\rangle = \mathsf{npp0.5+}$ (channels dictionary)
anzStreuBases	nbr. of bases grown from different initial seed bases
CgfCycles	nbr. of cycles each cfg. $\in$ bastypes is optimized
nRaces	nbr. of generations for each CgfCycle
cradleCapacity	nbr. of children produces within a Race
ini_grid_bounds	arg. of function `seedMat`; bounds of the initial, partially randomized geometric grid; 8-element array
ini_dims	arg. of function `seedMat`; nbr. of width parameters per cfg. for Jacobi 1,2 ($\gamma_{1,2}$); 1st pair: initial state; 2nd pair: final state
minCond	minimal condition number=ratio between absolute values of the smallest and largest norm eigenvalue;
denseEVinterval	parameter to det. loveliness of a vector in `loveliness` and `basQ` in `genetic_width_growth.py`
removalGainFactor	while stabilizing the initial seed basis and purging an optimized basis after CfgCycles of idlers, the removal of one of the latter must increase the quality by this factor
maxOnPurge	max. nbr. of basis vectors tested for their effect on stability; ideally $=\mathsf{dim}$(basis)
maxOnTrail	max. nbr. of basis vectors tested for their effect on quality; ideally $=\mathsf{dim}$(basis)
muta_initial	mutation rate (random bit flip) during offspring generation
output	**written in `respath` (set in `bridgeA3.py`)**
Ssigbasv3heLIT_Jpi_BasNR-<basisSet>.dat	FORTRAN bookkeeping
SLITbas_full_Jpi_BasNR-rndSet .dat	*
Ssigbasv3heLIT_Jpi .dat	*
SLITbas_full_Jpi .dat	*
mat_Jpi_BasNR-rndSet	Norm: $\mathbb{N} = \langle\, \Phi_i \mid \Phi_j \,\rangle / \sqrt{\langle\, \Phi_i \mid \Phi_i \,\rangle \cdot \langle\, \Phi_j \mid \Phi_j \,\rangle}$ Hamiltonian: $\mathbb{H} = \left\langle\, \Phi_i \,\middle\vert\, \hat{H} \,\middle\vert\, \Phi_j \,\right\rangle / \sqrt{\langle\, \Phi_i \mid \Phi_i \,\rangle \cdot \langle\, \Phi_j \mid \Phi_j \,\rangle}$; $\mathbb{H}$ is specified in `bridgeA3.py` with potnn(n), tnni $\mathbb{N}$ is normalized such that its diagonal $= \mathbb{1}$; ECCE units: $[\mathbb{N}_{ij}] = 0$ $[\mathbb{H}_{ij}] = \left[\hat{H}\right] = \mathsf{MeV}$

2. calculate the overlap matrix elements

calculation flow step (5)

`A3_lit_M.py`

argument	comment
`multiplicity` L	$j_L(kr_i)Y_{LM}(\hat{\boldsymbol{r}}_i)$ with photon energy k ()
output	written in `respath` (set in `bridgeA3.py`)
`componentN_S_finalJ_finalMJ_multipoleM`	

3.

b. Quantity of interest . . . .

The result of the following steps is the part of the Compton-scattering amplitude (eq. (2) in ref. [1])

$$T^{if}_{\lambda'\lambda}\left(\boldsymbol{k}',\boldsymbol{k}\right)\quad\text{with}\quad\begin{cases}\lambda'(\lambda) & \text{out-(in-)going photon polarization } \boldsymbol{e}_\lambda\\ \boldsymbol{k}'(\boldsymbol{k}) & \text{out-(in-)going photon 3-momentum}\\ i(f) & \text{quantum numbers of the initial(final) nuclear target}\end{cases}\quad;\tag{1}$$

with an intermediate, zero-photon state with energy $\omega + E_i$.

c. Basis optimization . . . .

Initial and final nuclear states are expanded in a non-orthonormal basis. The expansion should approximate physical features of these states relevant at the scales at which the amplitude is to be calculated. This scale determines the coupling mechanism to the electromagnetic field, and demands a more or less accurate description of the nuclear state. But this is a different story, while the details of

$$\left\langle\,\underline{\boldsymbol{\rho}}\mid J^\pi\,\right\rangle = \sum_n c_n\,\Phi^{\mathrm{RGM}}_{n,\pi,[L_n\otimes S_n]^J}\quad\text{with}\quad\begin{cases}[L_n\otimes S_n]^J & \textit{i.e.}\text{ , LS-coupling scheme}\\ \underline{\boldsymbol{\rho}} & \text{set of } A-1 \text{ 3-d Jacobi vectors}\\ J,\pi & \text{total angular momentum, parity of the state}\end{cases}\quad;\tag{2}$$

and a decomposition which couples orbital- and spin-angular momenta

$$\Phi^{\mathrm{RGM}}_{n,\pi,[L_n\otimes S_n]^J} = \left[\phi_n\otimes\Xi_n\right]^J\cdot\mathcal{T}_n\tag{3}$$

are to be set, here. The orbital part, ϕ of Φ is

$$\phi_n = \prod_{i=1}^{A-1} e^{-\gamma_{n,i}\boldsymbol{\rho}_i^2}\cdot\mathcal{Y}_{l_{n,i}m}(\boldsymbol{\rho}_i)\tag{4}$$

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basis parameter	implementation	comment
S_n		total spin **and** all intermediate couplings
-	`bridgeA3.py`	spin-orbital configuration combinations considered in $\left\vert\,{}^3\mathrm{He}\,\right\rangle$ and $\hat{\mathcal{O}}_{pq}\otimes\left\vert\,{}^3\mathrm{He}\,\right\rangle$
-	`three_particle_functions.py`	dictionary `elem_spin_prods_3` translates, *e.g.* , `he_no1` $\rightarrow$ $\left[\left[\sigma_1\otimes\sigma_2\right]^{s_{12}=1}\otimes\sigma_3\right]^{S=1/2}\cdot\left[\left[\tau_1\otimes\tau_2\right]^{\tau_{12}=0}\otimes\tau_3\right]^{S=1/2}$

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