Connecting R-matrix phenomenology to *ab initio* approaches

NSAC Long Range Plan Town Hall Meeting
Nuclear Structure, Reactions & Astrophysics

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Motivation

Evaluated nuclear data & resonance parametrization

Smooth (differentiable) representation of scattering/reaction data is important for a variety of applications

- Nuclear astrophysics & cosmology
- Neutrinos and fundamental symmetries
- Energy
- Nuclear criticality & safety
- Nuclear security

Resonance parameters are compact, concise representation of the data that are calculable

- Phenomenologically
- *Ab initio*

Resonance parameters

- What do they parametrize?
  - Analytic features of the *T* matrix
    - Poles [& branch points]
- **Model independent** representations of reaction/scattering data
- **Resolvent formalism** unifies various parametrizations
  - *S* or *T* matrix poles
  - Brune alternative
  - …
  - **NB:** Breit-Wigner parameters are not on the list
    - unconstrained by unitarity, causality, etc.

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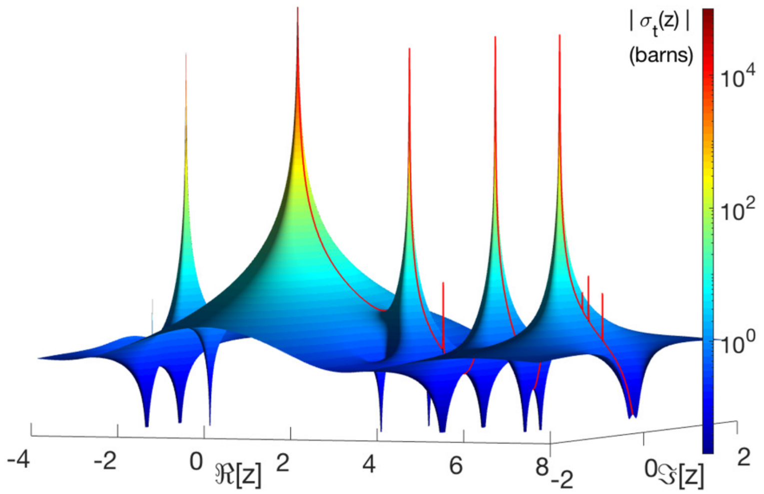

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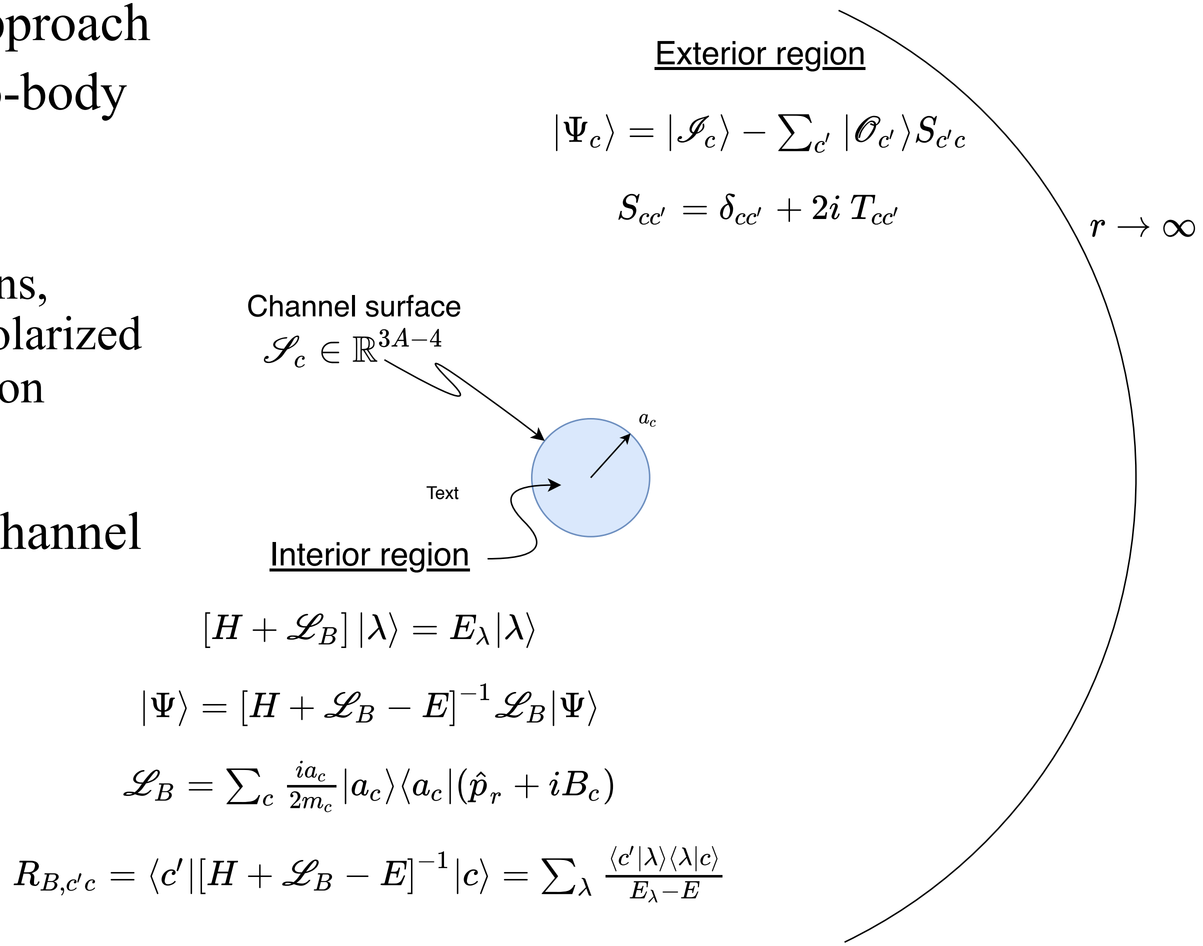
R-matrix method

Phenomenology

- Model-independent representation of the data
- Comprehensive & unified approach
  - respects multichannel two-body unitarity & causality
  - all data
    - total cross section, reactions, angular distributions, unpolarized and polarization information
- Compact
  - # parameters linear with channel space dimension
- Meromorphic
  - branch points *factorize*



Uncertainty quantification

$$\chi^2_{\mathrm{EDA}}(\mathbf{p}) = \sum_{M,i_M} \left[\frac{n_{i_M} X_{i_M}(\mathbf{p}) - R_{i_M}}{\delta R_{i_M}}\right]^2 + \left[\frac{n_M S_M - 1}{\delta S_M / S_M}\right]^2 \left\{ \begin{array}{rl} M & : \text{experimental setup} \\ i & : \text{observable} \\ R_{i_M}, \delta R_{i_M} & : \text{relative measurement, uncert.} \\ X_{i_M} & : \text{calc'd observable} \\ n_M & : \text{normalization} \end{array} \right.$$

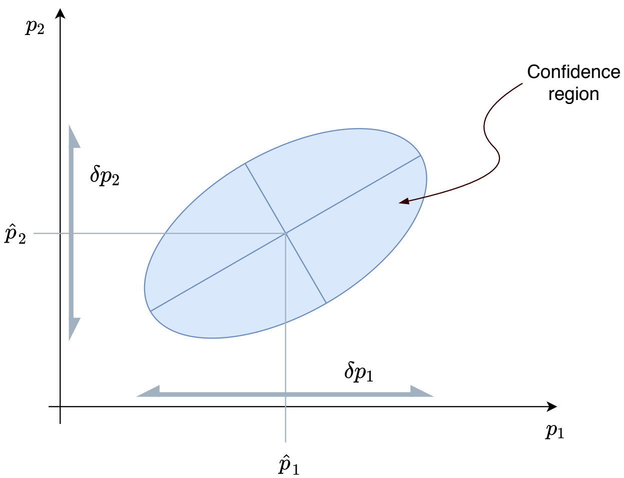
Uncertainty determination comparison:

1) previous: $\delta\chi^2 = 1 \implies$ Uncertainties too small; scaling: $\delta p_i = (C^0_{ii})^{1/2} \sim \mathcal{O}(N_p^{-1/2})$

2) improved:

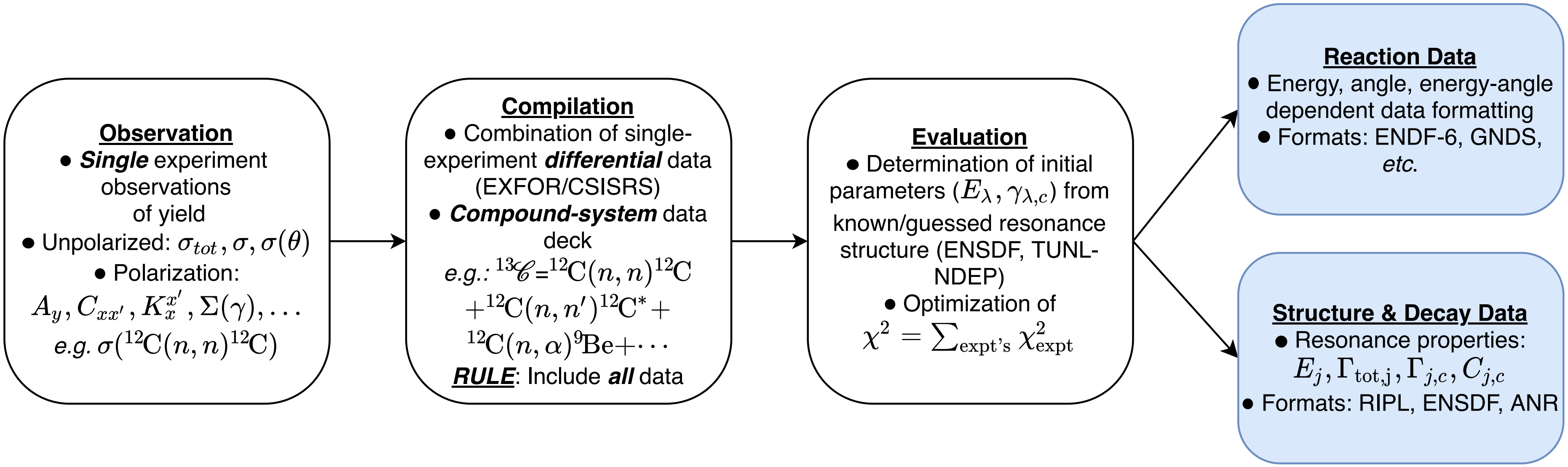
$$P(\delta\chi^2 | k \text{ DOF}) = \frac{1}{2^{k/2}\Gamma(k/2)} \int_0^{\delta\chi^2} dt\, t^{k/2-1} e^{-t/2} = \mathrm{CL}(68\%: 1-\sigma;\ 95\%: 2-\sigma; \ldots)$$

Better scaling: $\delta p_i \sim (N_p C_{ii})^{1/2}$



Nuclear data evaluation workflow

R-matrix example



- Four phases of Evaluation
  - Assess single experiment observables
  - Compile all process (total, elastic, inelastic, reaction, polarization)
  - Model / parametrization fitting
  - Production of **Reaction Data** and **Structure & Decay Data**

R-matrix method

Ab initio

- Two approaches
  - Solve many-body Schrodinger subject to Hermitian BC at finite radius
  - Or solve for generalized Green function

$$\left[H + \hat{\mathscr{L}}\right]|\lambda\rangle = E_\lambda|\lambda\rangle,$$

$$|F\rangle = |f\rangle + A|a\rangle$$

$$|\Psi\rangle = \left(H + \mathscr{L}_a^{(0)} - E\right)^{-1}|F\rangle \quad \Longleftrightarrow \quad \begin{aligned} (H-E)\,\Psi(r) &= f(r) \\ \left(\frac{d}{dr} - ik\right)(r\Psi(r))\Big|_{r=a} &= A \end{aligned}$$

$$\mathscr{L}_a^{(0)} = \frac{i\hbar}{2\mu}|a\rangle\langle a|\hat{p}_r$$

$$\Psi(r) = \int dr' r'^2 G(r,r')F(r')$$

- Compare resonance parameters from *ab initio* approaches against the phenomenology

$$S = e^{-2ika}\left[1 + \frac{ika^2}{m}\langle a|\left(H + \mathscr{L}_a(k) - E\right)^{-1}|a\rangle\right]$$

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda,c}\gamma_{\lambda,c'}}{E - E_\lambda}$$

Thanks in advance for your questions & support