TRIUMF

Ab initio investigation of the $^{12}C(n,p)^{12}B$ charge-exchange reaction

The 7th international workshop on Compound-Nuclear Reactions and Related Topics (CNR*24)

Vienna International Centre, IAEA
July 8th, 2024

Petr Navratil

TRIUMF

2024-07-06

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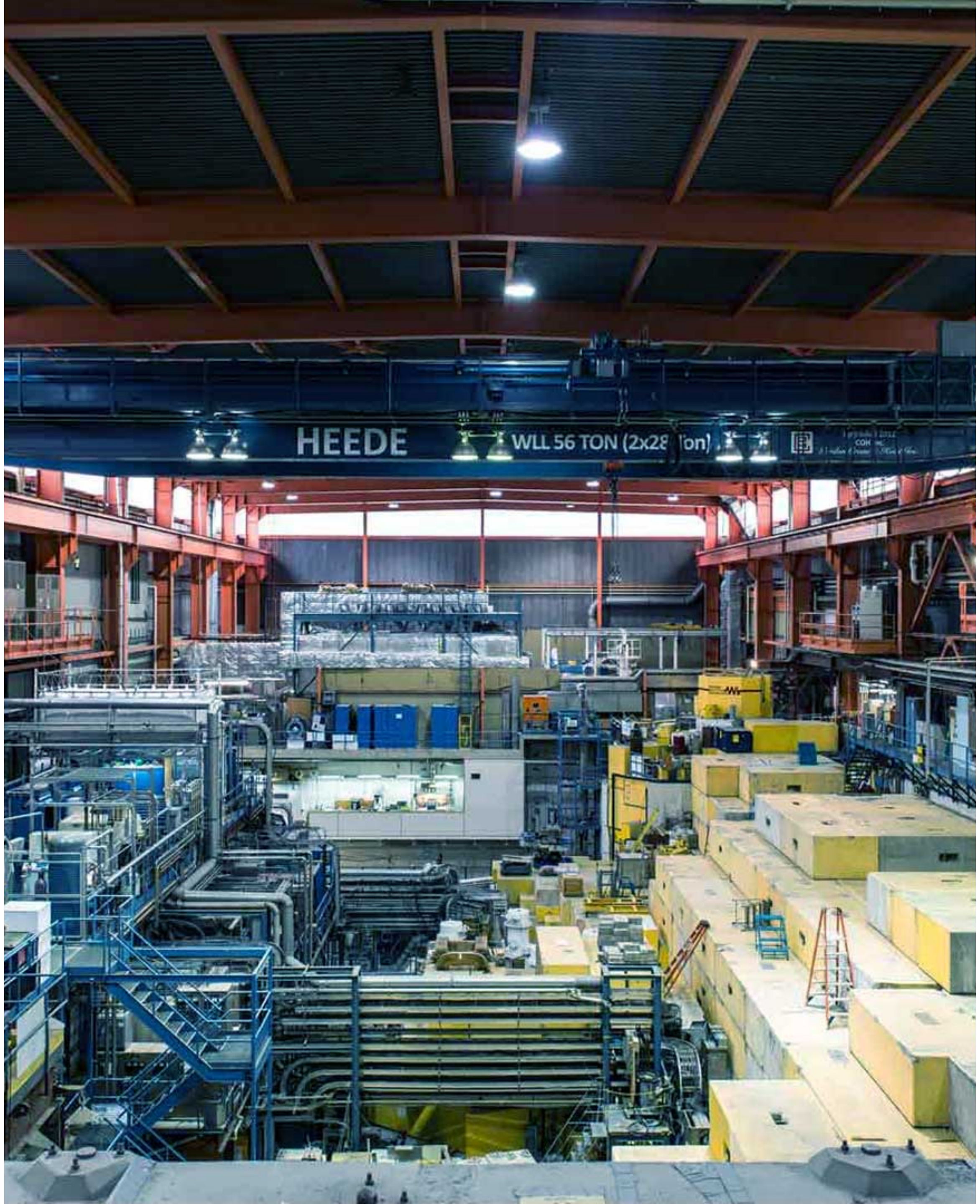
Discovery, accelerated

Outline

- *Ab initio* nuclear theory
  - No-core shell model (NCSM) and NCSM with continuum (NCSMC)
    - Input chiral NN+3N interactions
- Charge exchange reactions in NCSMC
  - $^{12}C(n,p)^{12}B$

TRIUMF

Ab initio nuclear theory



Discovery, accelerated

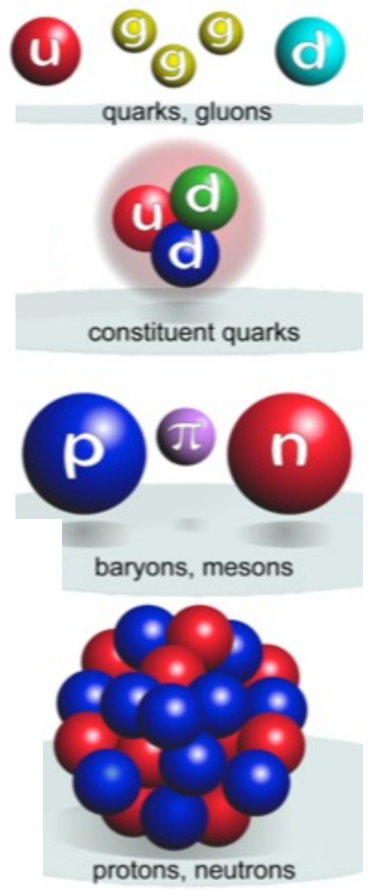
First principles or *ab initio* nuclear theory

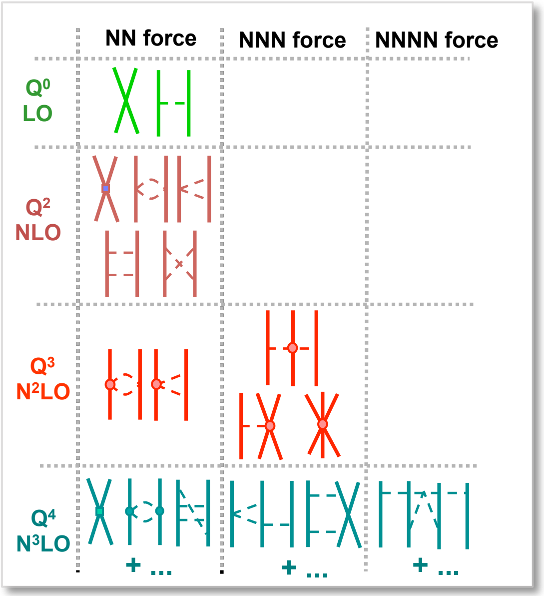
Quantum Chromodynamics (QCD)

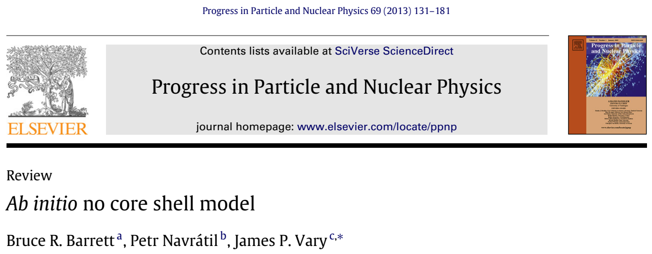
Chiral Effective Field Theory (parameters fitted to NN data)

Current *ab initio* nuclear theory

$$H\,\Psi^{(A)} = E\,\Psi^{(A)}$$



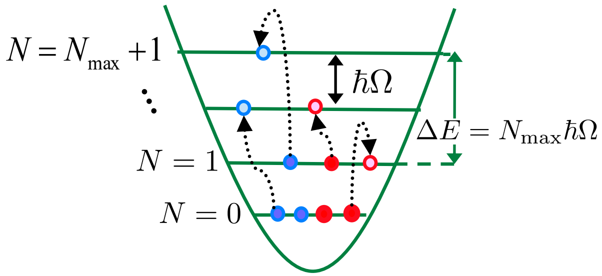


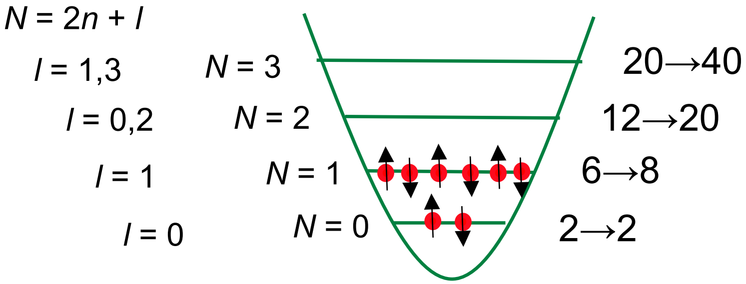


Ab initio No-Core Shell Model (NCSM)

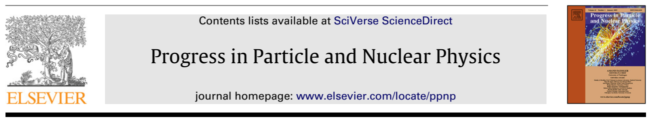
- Basis expansion method
  - Harmonic oscillator (HO) basis truncated in a particular way (N_{max})
  - Why HO basis?
    - Lowest filled HO shells match magic numbers of light nuclei (2, 8, 20 – ^{4}He, ^{16}O, ^{40}Ca)
    - Equivalent description in relative(Jacobi)-coordinate and Slater determinant (SD) basis
- Short- and medium range correlations
- Bound-states, narrow resonances

NCSM





$E = (2n + l + \frac{3}{2})\hbar\Omega$


Progress in Particle and Nuclear Physics 69 (2013) 131–181
Contents lists available at SciVerse ScienceDirect
Progress in Particle and Nuclear Physics
journal homepage: www.elsevier.com/locate/ppnp
Review
Ab initio no core shell model
Bruce R. Barrett[a], Petr Navrátil[b], James P. Vary[c,*]

Ab initio No-Core Shell Model (NCSM)

NCSM

- Basis expansion method
  - Harmonic oscillator (HO) basis truncated in a particular way (N_{max})
  - Why HO basis?
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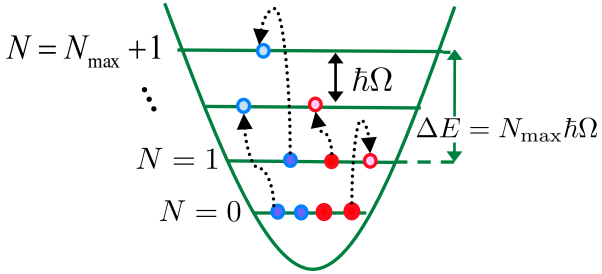
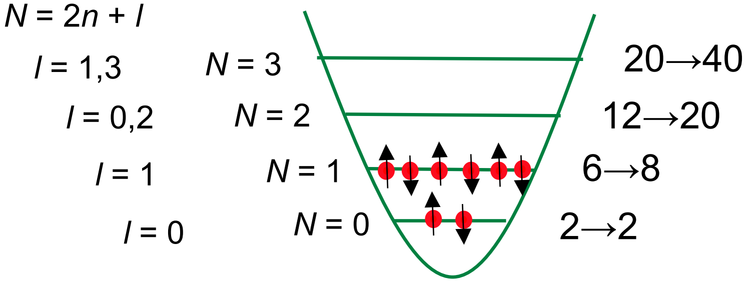


$$\Psi^A = \sum_{N=0}^{N_{max}} \sum_i c_{Ni} \Phi_{Ni}^{HO}(\vec{\eta}_1, \vec{\eta}_2, \ldots, \vec{\eta}_{A-1})$$

$$\Psi_{SD}^A = \sum_{N=0}^{N_{max}} \sum_j c_{Nj}^{SD} \Phi_{SD\,Nj}^{HO}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = \Psi^A \varphi_{000}(\vec{R}_{CM})$$



$$E = (2n + l + \tfrac{3}{2})\hbar\Omega$$

Ab Initio Calculations of Structure, Scattering, Reactions

Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)} , \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \; \gamma_{\nu}(\vec{r}\,) \; \hat{A}_{\nu} \left| {}_{(A-a)} \; \vec{r} \; {}_{(a)} \; , \nu \right\rangle$$

S. Baroni, P. Navratil, and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

Ab Initio Calculations of Structure, Scattering, Reactions

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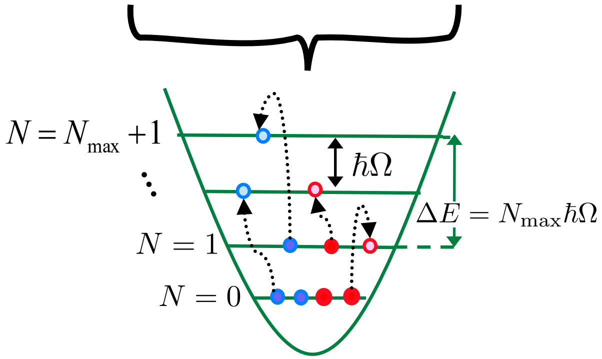

Static solutions for aggregate system,
describe all nucleons close together

S. Baroni, P. Navratil, and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

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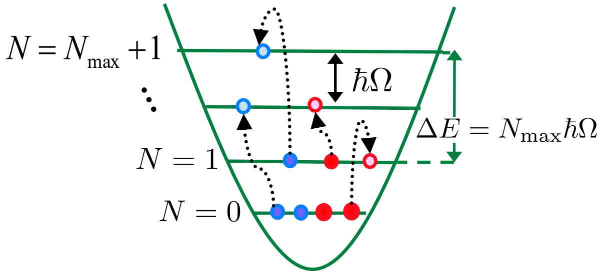


Static solutions for aggregate system, describe all nucleons close together

Continuous microscopic cluster states, describe long-range projectile-target

S. Baroni, P. Navratil, and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

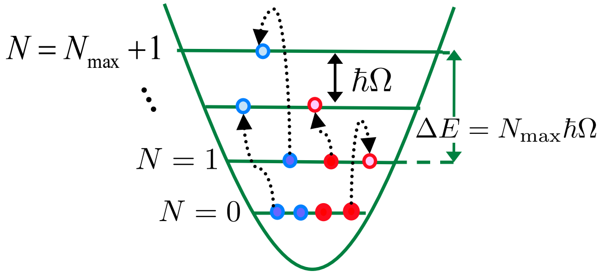
Ab Initio Calculations of Structure, Scattering, Reactions

Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)

Unknowns

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)} , \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r}\,)\; \hat{A}_{\nu} \left| {}_{(A-a)} \;\; \vec{r} \;\; (a) \, , \nu \right\rangle$$



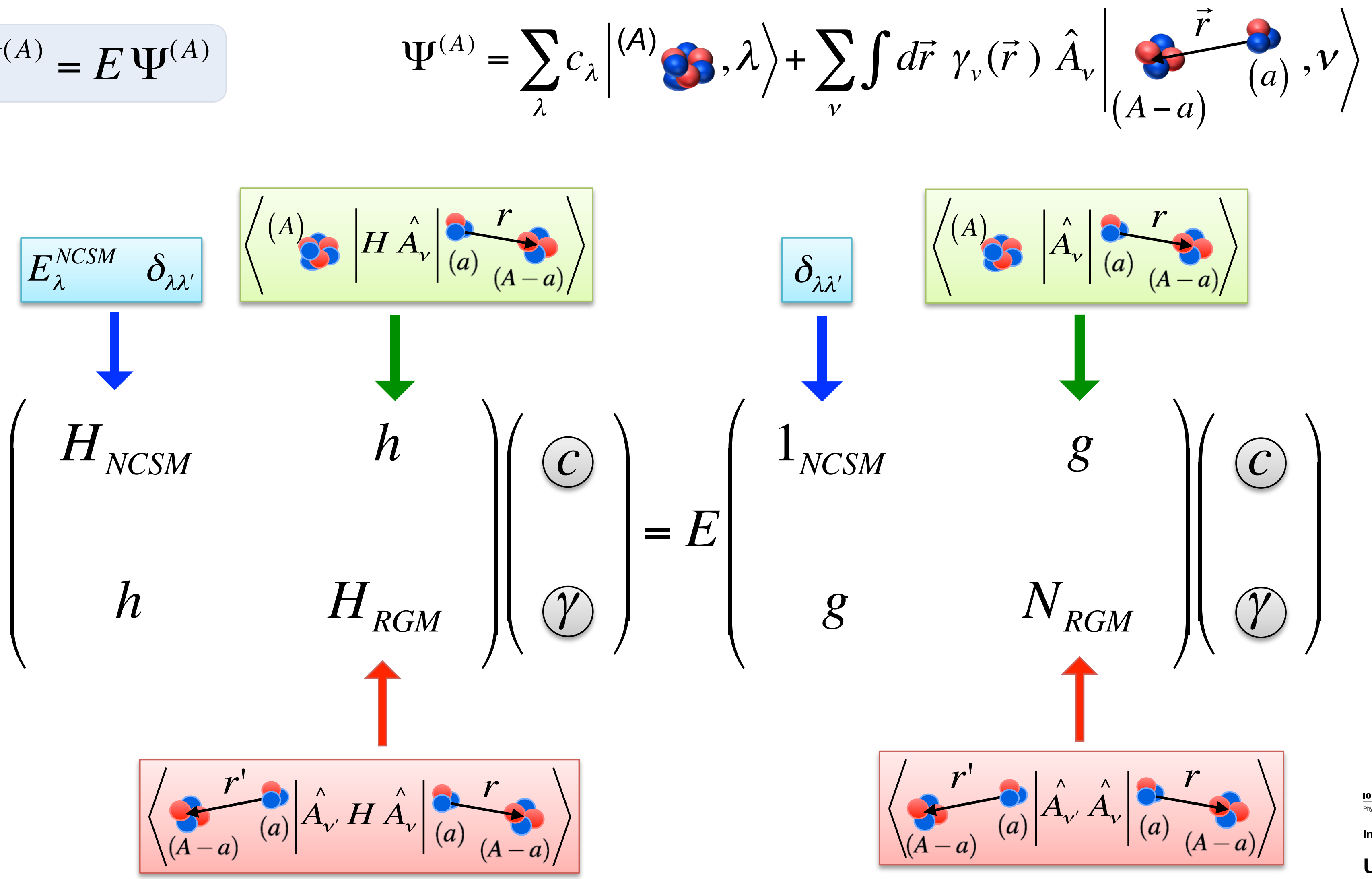
Static solutions for aggregate system, describe all nucleons close together

Continuous microscopic cluster states, describe long-range projectile-target

S. Baroni, P. Navratil, and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

Coupled NCSMC equations

$$H\,\Psi^{(A)} = E\,\Psi^{(A)}$$



IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta
Phys. Scr. 91 (2016) 053002 (38pp) doi:10.1088/0031-8949/91/5/053002

Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]

PHYSICAL REVIEW C **101**, 014318 (2020)

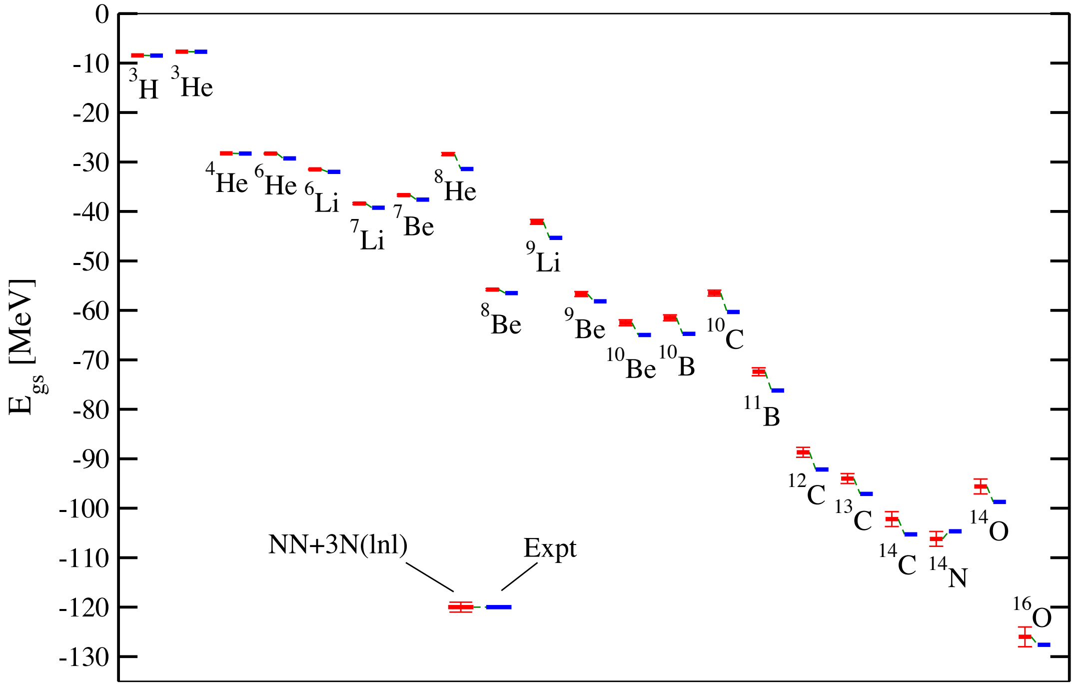
Novel chiral Hamiltonian and observables in light and medium-mass nuclei

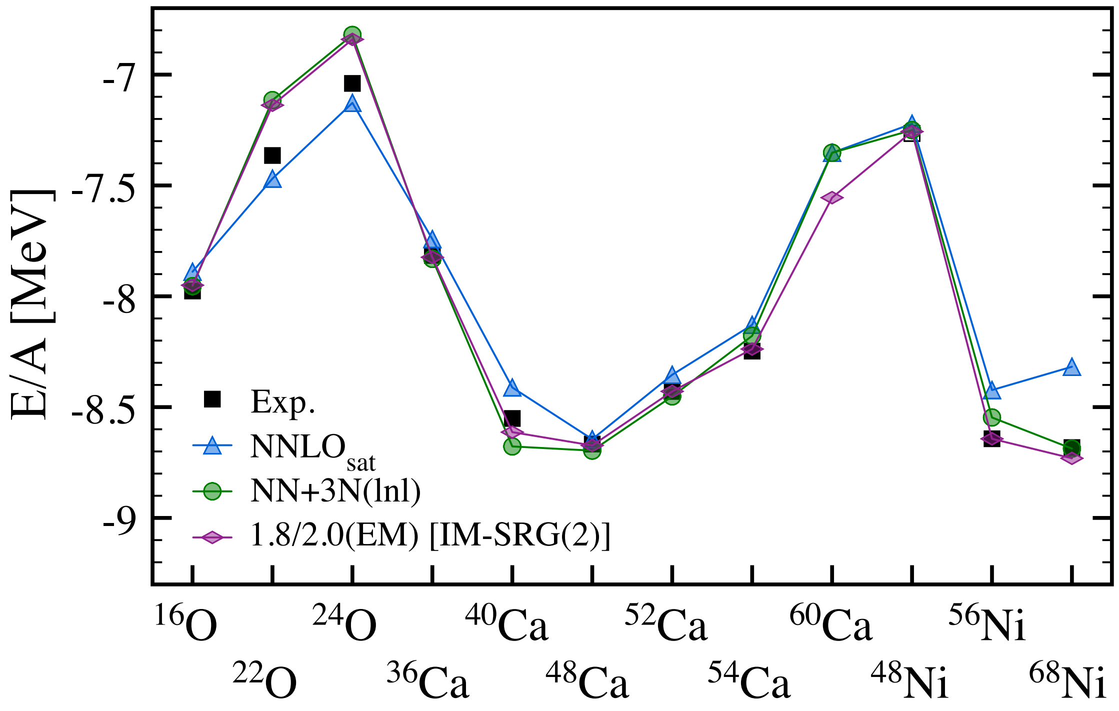
V. Somà,[1,*] P. Navrátil,[2,†] F. Raimondi,[3,4,‡] C. Barbieri,[4,§] and T. Duguet[1,5,‖]

Input for NCSMC calculations: Nuclear forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - **The Hamiltonian fully determined in *A*=2 and *A*=3,4 systems**
    - Nucleon–nucleon scattering, deuteron properties, ^{3}H and ^{4}He binding energy, ^{3}H half life
  - Light nuclei – NCSM
  - Medium mass nuclei – Self-Consistent Green's Function method

NN N^{3}LO (Entem-Machleidt 2003)
3N N^{2}LO w local/non-local regulator





1.8/2.0 (EM) results: J. Simonis, S. R. Stroberg, K. Hebeler, J. D. Holt, and A. Schwenk, Phys. Rev. C 96, 014303 (2017).

Recently developed NCSMC capability – charge-exchange reaction calculations

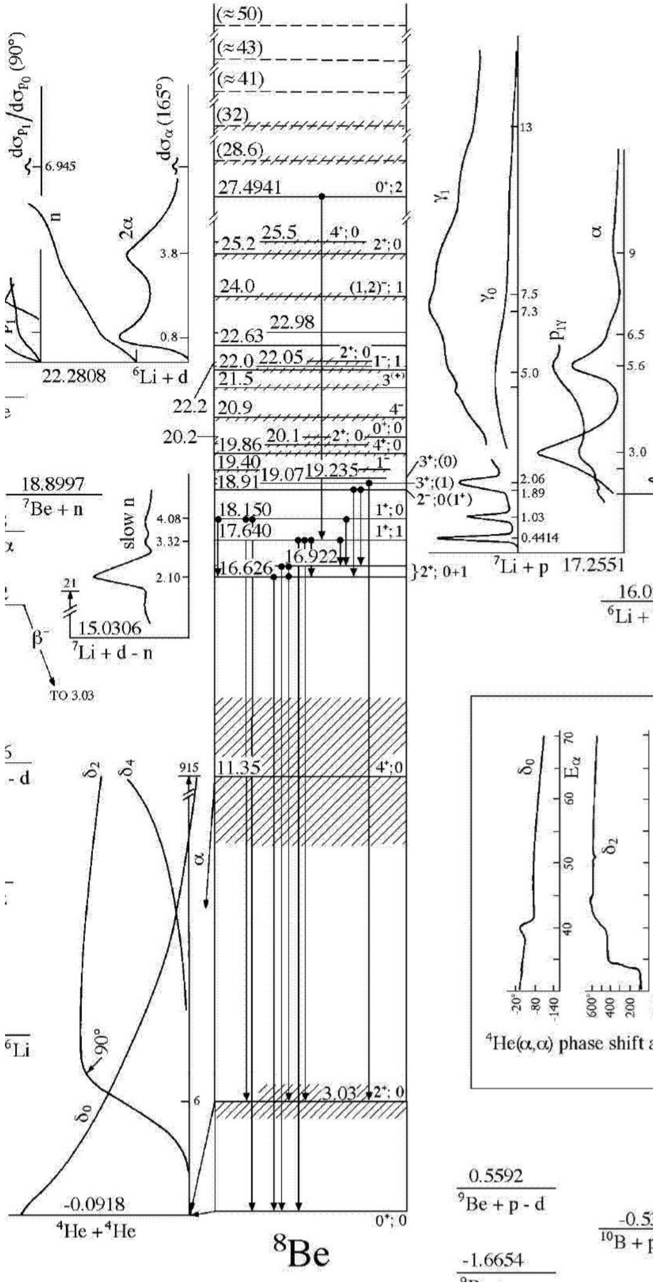
- The first published application - ^{7}Li+p scattering and radiative capture
  - Wave function ansatz

$$\Psi^{(8)}_{\text{NCSMC}} = \sum_{\lambda} c_\lambda \left|{}^8\text{Be}, \lambda\right\rangle + \sum_{\nu} \int dr \gamma_\nu(r) \hat{A}_\nu \left|{}^7\text{Li} + p, \nu\right\rangle + \sum_{\mu} \int dr \gamma_\mu(r) \hat{A}_\mu \left|{}^7\text{Be} + n, \mu\right\rangle$$

***Ab initio* investigation of the $^7\text{Li}(p, e^+e^-)^8\text{Be}$ process and the X17 boson**

P. Gysbers[1,2], P. Navrátil[1], K. Kravvaris[3], G. Hupin[4], S. Quaglioni[3]

arXiv:2308.13751 – Physical Review C, in press

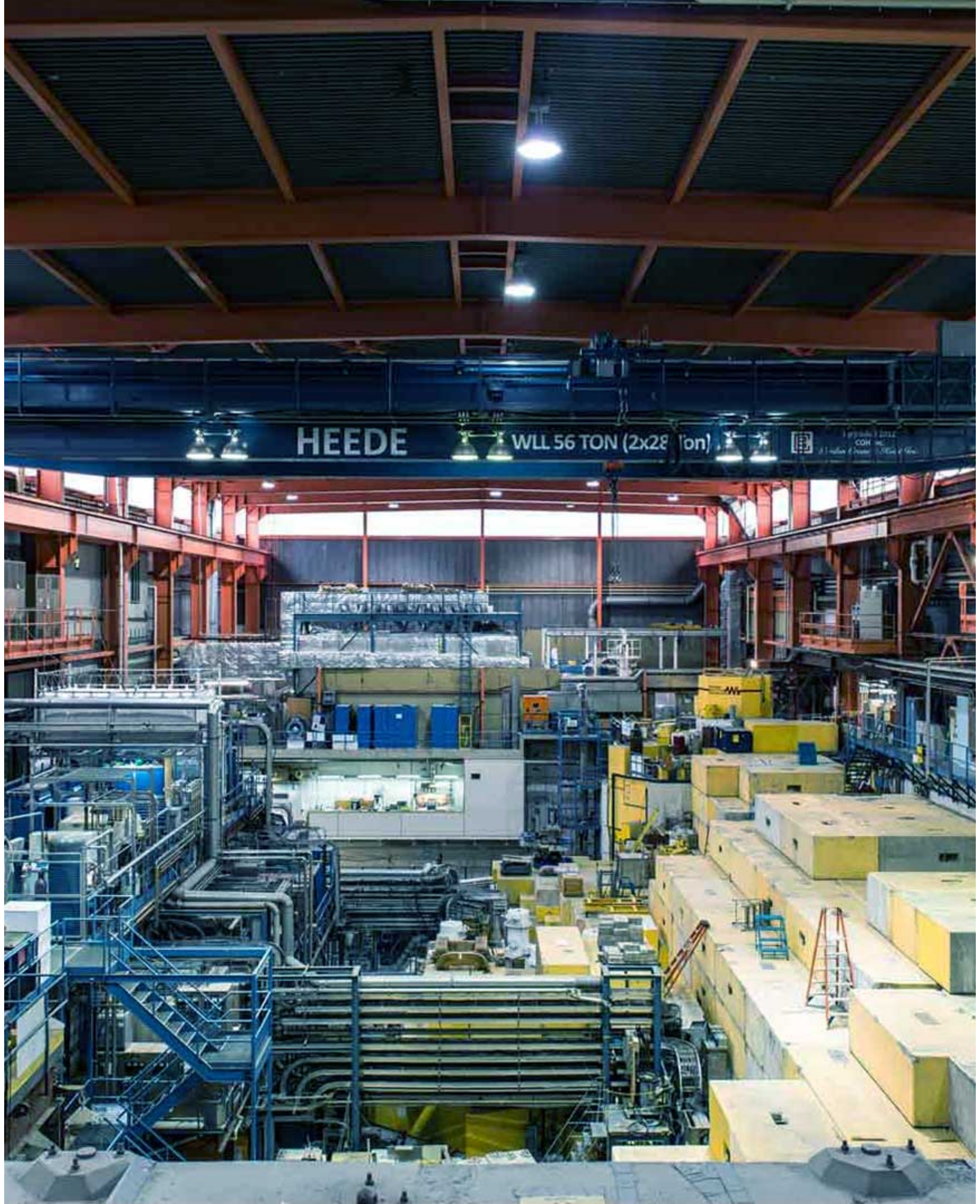


TRIUMF

$^{12}C(n,p)^{12}B$

In collaboration with
Matteo Vorabbi (U Surrey)

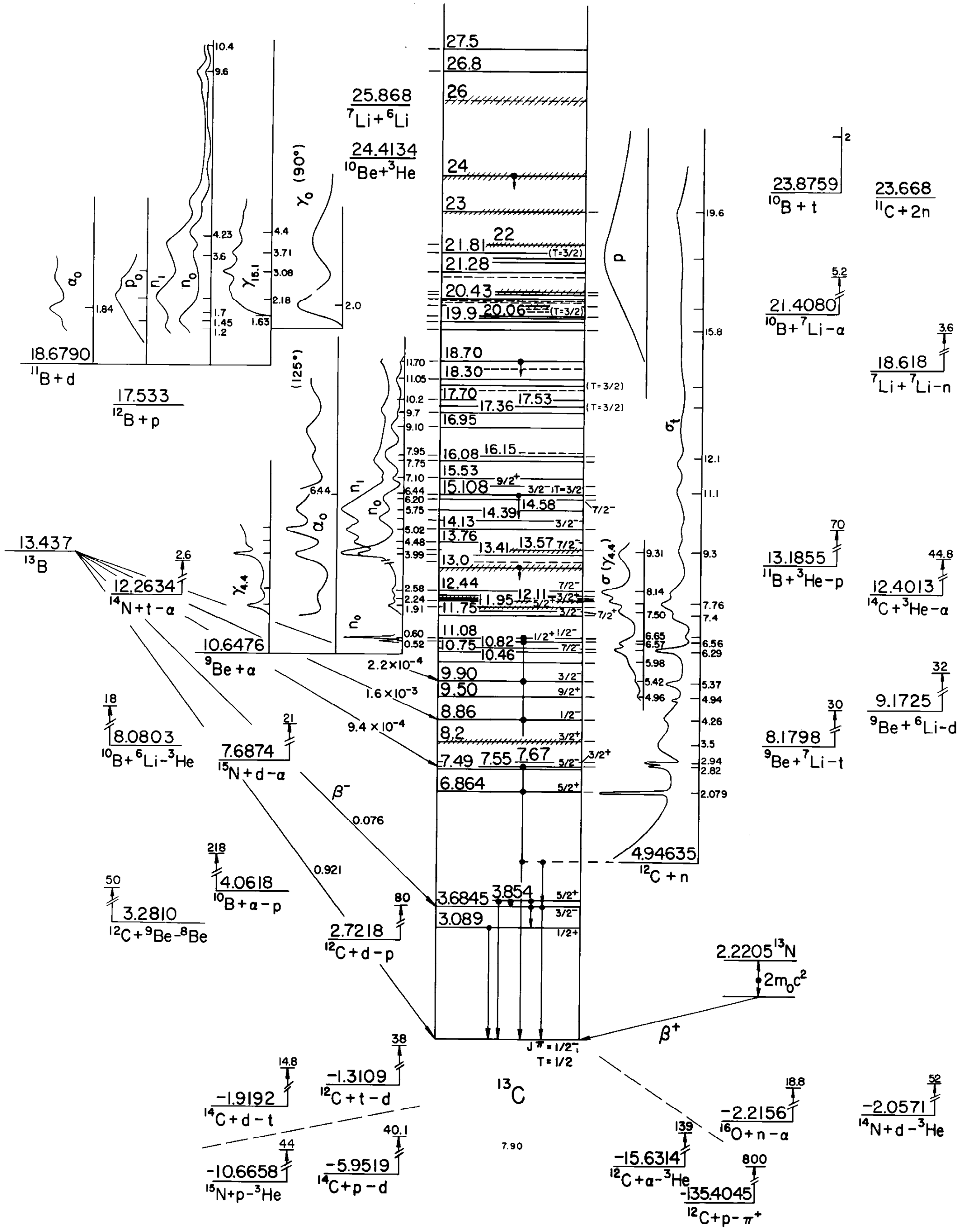
Calculations preliminary



Discovery, accelerated

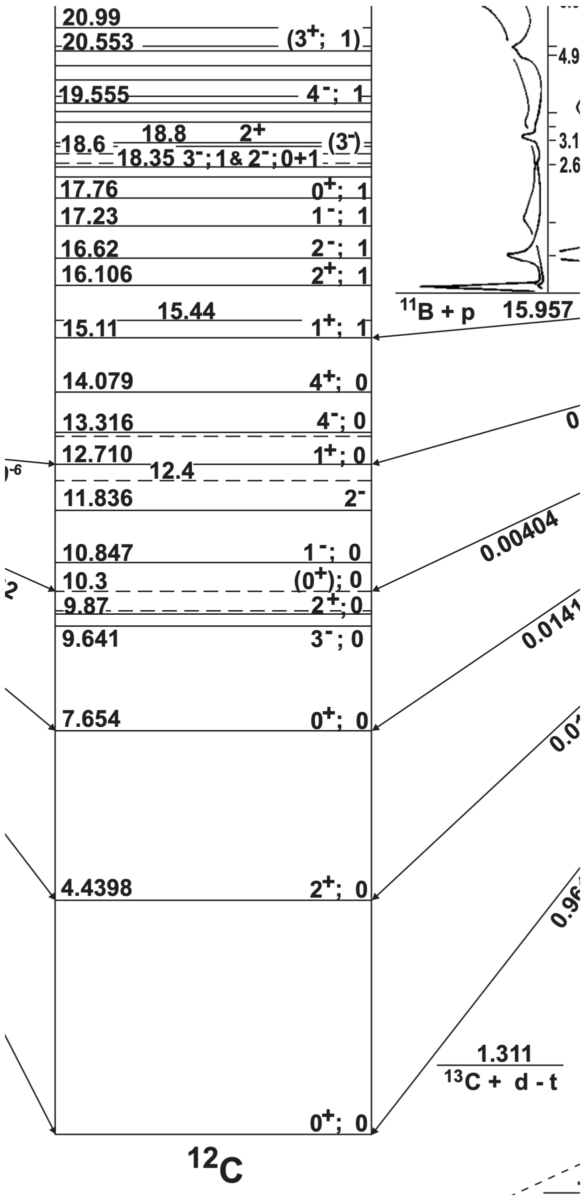
Motivation – characterization of single crystal diamond detectors, measurements at n-TOF at CERN

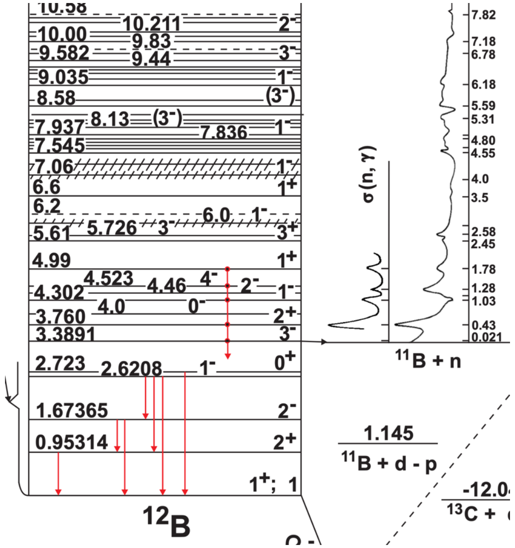
- High-energy neutron detection
  - Single crystal diamond detectors can be used in harsh environments – fusion reactor, have low gamma sensitivity
  - Neutron cross sections on carbon important in general
- (n,p) and (n,d) reactions on carbon measured at n-TOF (neutron-time-of-flight) facility at CERN
  - Measurements at two angles, no information on the final state excitation, E_n up to 26 MeV (24 MeV in CM)
  - For the cross-section determination, theoretical angular distributions needed including for the final nucleus excited states
- Apply NCSMC to $^{12}C(n,p)^{12}B$



^{13}C and ^{12}C(n,p)^{12}B in NCSMC

- Input - chiral NN N^{4}LO + 3N$_{lnl}$ interaction – SRG evolved
- Basis
  - ^{12}C 0$^+$ and 2$^+$ states (T=0)
  - ^{12}B 1$^+$ and 2$^+$ states (T=1)





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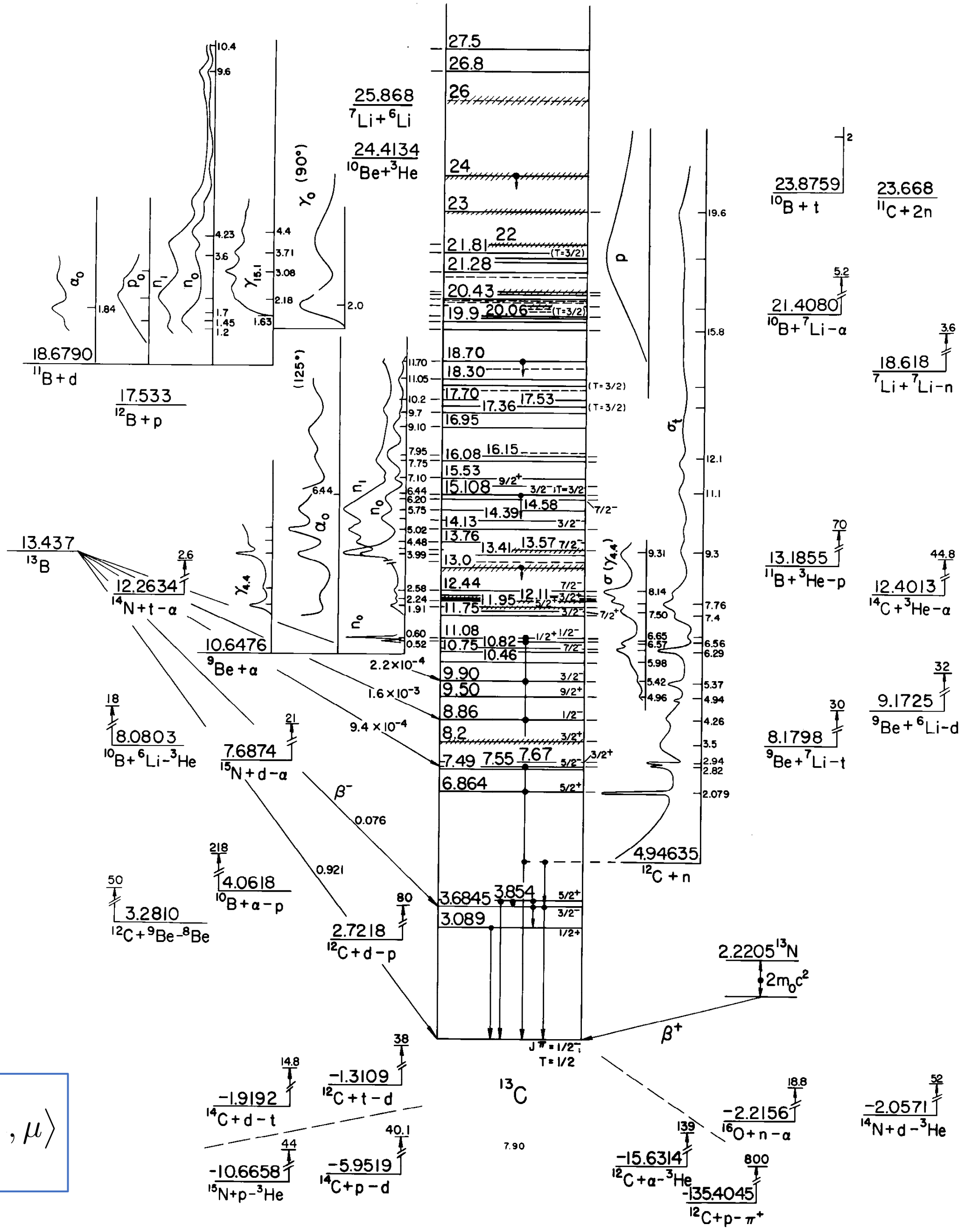
- Basis
  - ^{12}C 0$^+$ and 2$^+$ states (T=0)
  - ^{12}B 1$^+$ and 2$^+$ states (T=1)
  - ^{13}C
    - 24 negative-parity states – J=1/2$^-$ - 11/2$^-$
      - E$_x$ up to 24 MeV
    - 34 positive-parity states – J=1/2$^+$ - 11/2$^+$
      - E$_x$ up to 19 MeV



$$\Psi^{(13)}_{\text{NCSMC}} = \sum_\lambda c_\lambda \left| {}^{13}\text{C} \;\; \lambda \right\rangle + \sum_\nu \int dr\, \gamma_\nu(r) \hat{A}_\nu \left| {}^{12}\text{C+n} \;\; , \nu \right\rangle + \sum_\mu \int dr\, \gamma_\mu(r) \hat{A}_\mu \left| {}^{12}\text{B+p} \;\; , \mu \right\rangle$$

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      - E$_x$ up to 19 MeV

Very high density of states → difficult to converge by Lanczos iterations (>800, dim 186 million at N_{max}=7)

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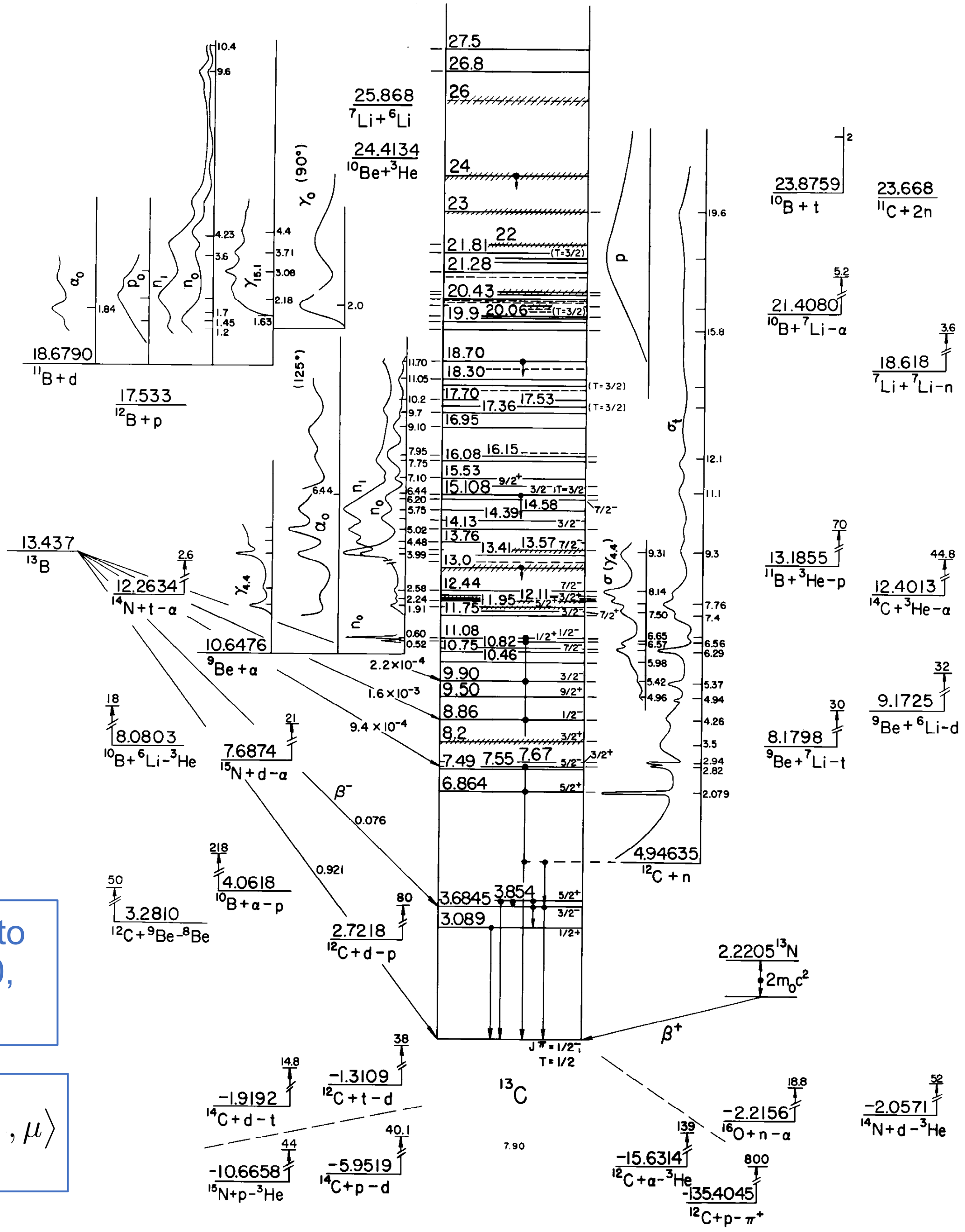
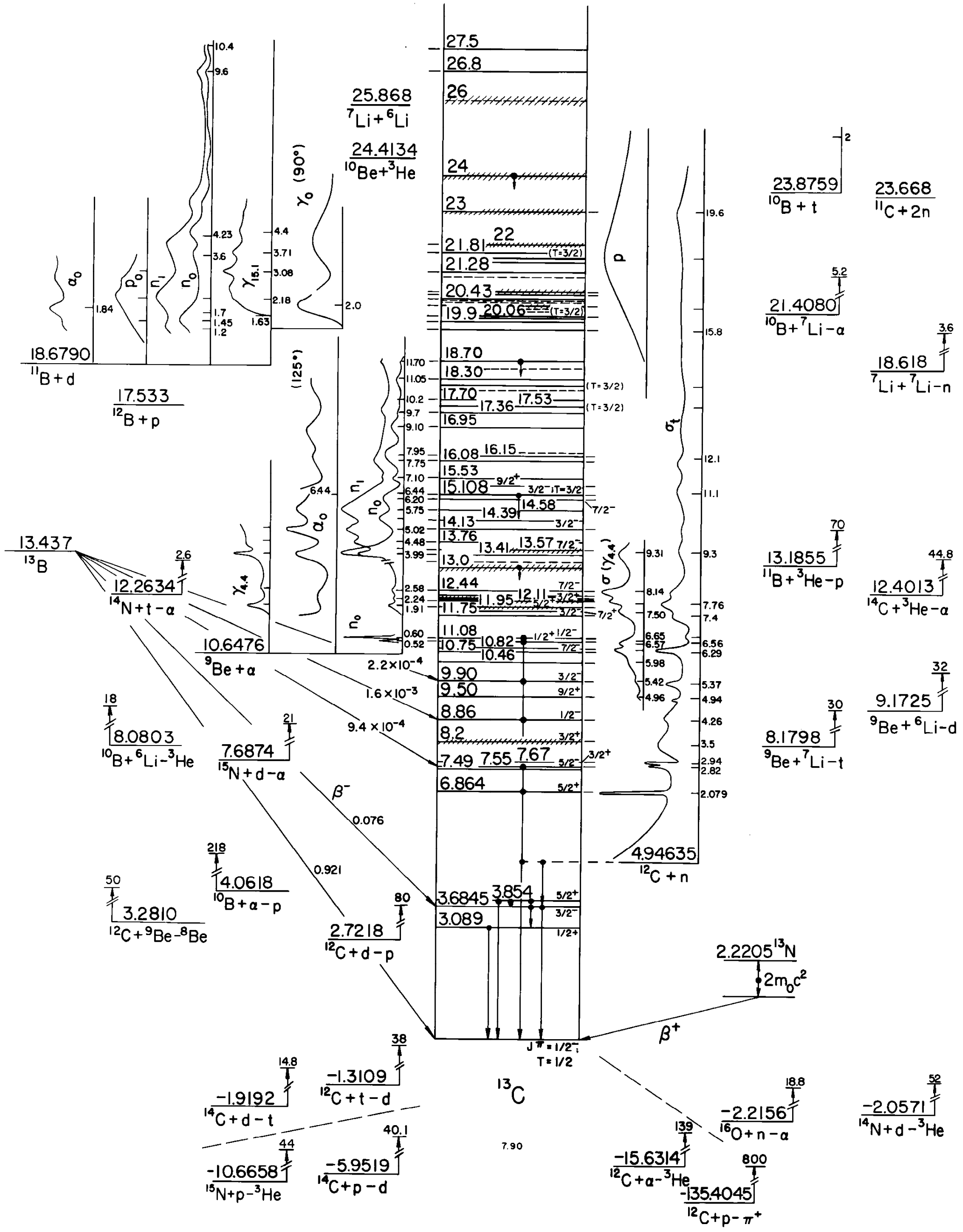


^{13}C and ^{12}C(n,p)^{12}B in NCSMC

- Input - chiral NN N^{4}LO + 3N$_{lnl}$ interaction – SRG evolved
- *Ab initio* results – N_{max}=7 (N_{max}=5 close to N_{max}=7)
  - Three bound states vs. four in experiment:
    - E(1/2$^-$) = -4.98 MeV vs. Expt. -4.95 MeV
    - E(1/2$^+$)= -0.77 MeV vs. Expt. -1.86 MeV
    - E(3/2$^-$) = -1.81 MeV vs. Expt. -1.26 MeV
    - E(5/2$^+$)= +0.33 MeV vs. Expt. -1.09 MeV



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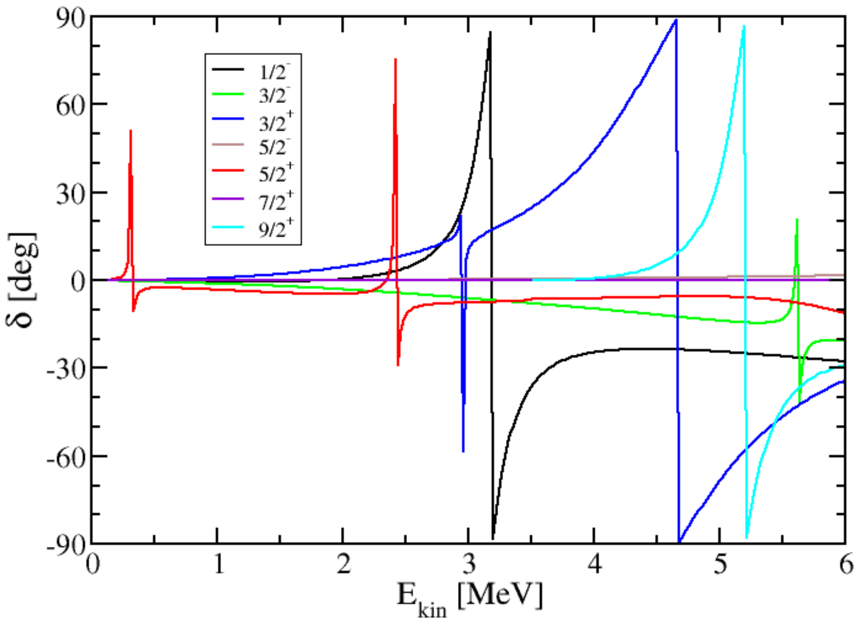
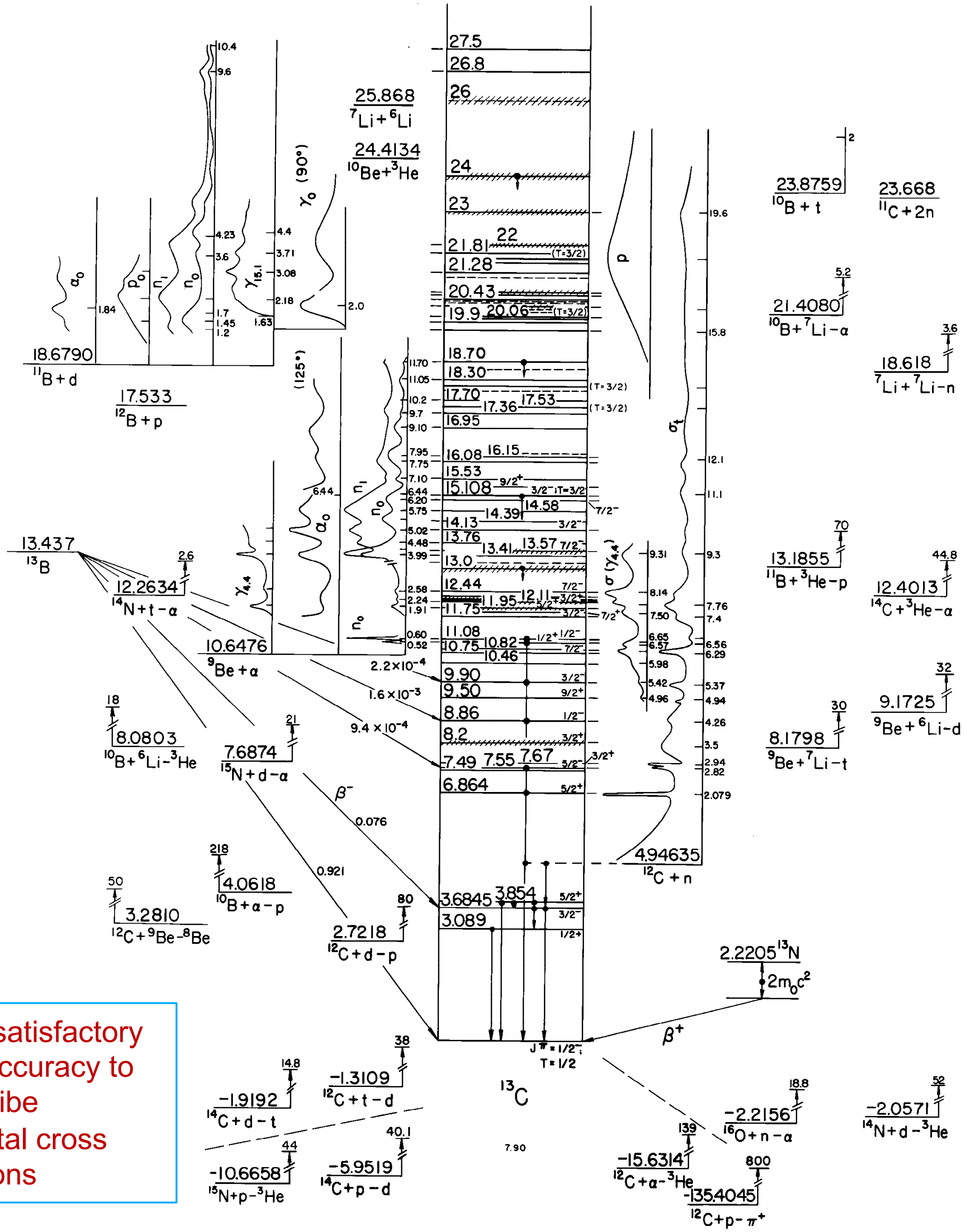
    - E(5/2$^+$)= +0.33 MeV vs. Expt. -1.09 MeV
  - Resonances



Qualitatively satisfactory
Insufficient accuracy to describe experimental cross sections



NCSMC phenomenology

$$H\,\Psi^{(A)} = E\,\Psi^{(A)} \qquad \Psi^{(A)} = \sum_\lambda c_\lambda \left|{}^{(A)}, \lambda\right\rangle + \sum_\nu \int d\vec{r}\; \gamma_\nu(\vec{r}\,)\; \hat{A}_\nu \left|\, \vec{r}\;\; {}_{(A-a)}\; (a), \nu \right\rangle$$

$$E_\lambda^{NCSM}\,\delta_{\lambda\lambda'} \qquad \left\langle {}^{(A)} \right| H\,\hat{A}_\nu \left| \overset{r}{(a)\;(A-a)} \right\rangle \qquad \delta_{\lambda\lambda'} \qquad \left\langle {}^{(A)} \right| \hat{A}_\nu \left| \overset{r}{(a)\;(A-a)} \right\rangle$$

$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

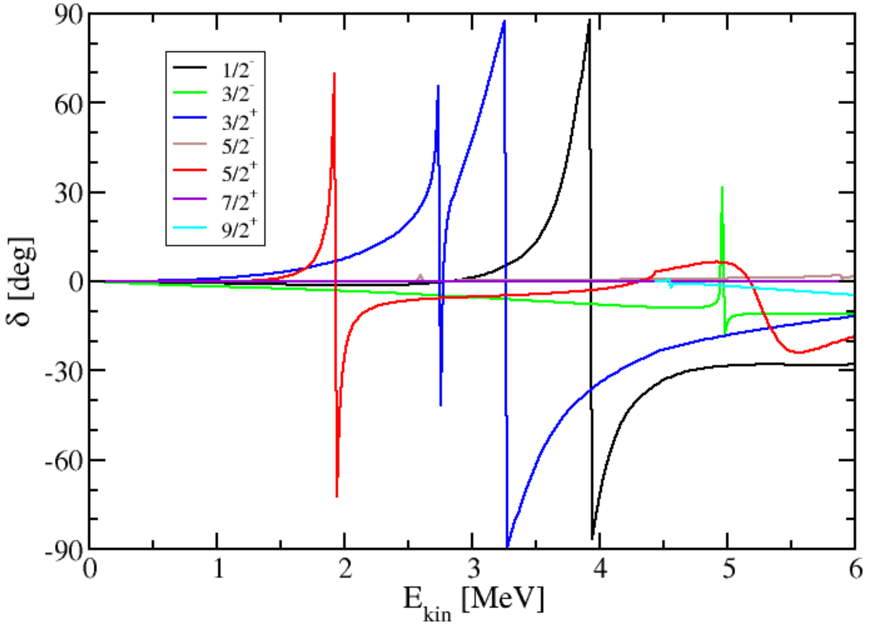
$$\left\langle \overset{r'}{(A-a)\;(a)} \right| \hat{A}_{\nu'}\,H\,\hat{A}_\nu \left| \overset{r}{(a)\;(A-a)} \right\rangle \qquad \left\langle \overset{r'}{(A-a)\;(a)} \right| \hat{A}_{\nu'}\,\hat{A}_\nu \left| \overset{r}{(a)\;(A-a)} \right\rangle$$

E_λ^{NCSM} energies treated as adjustable parameters

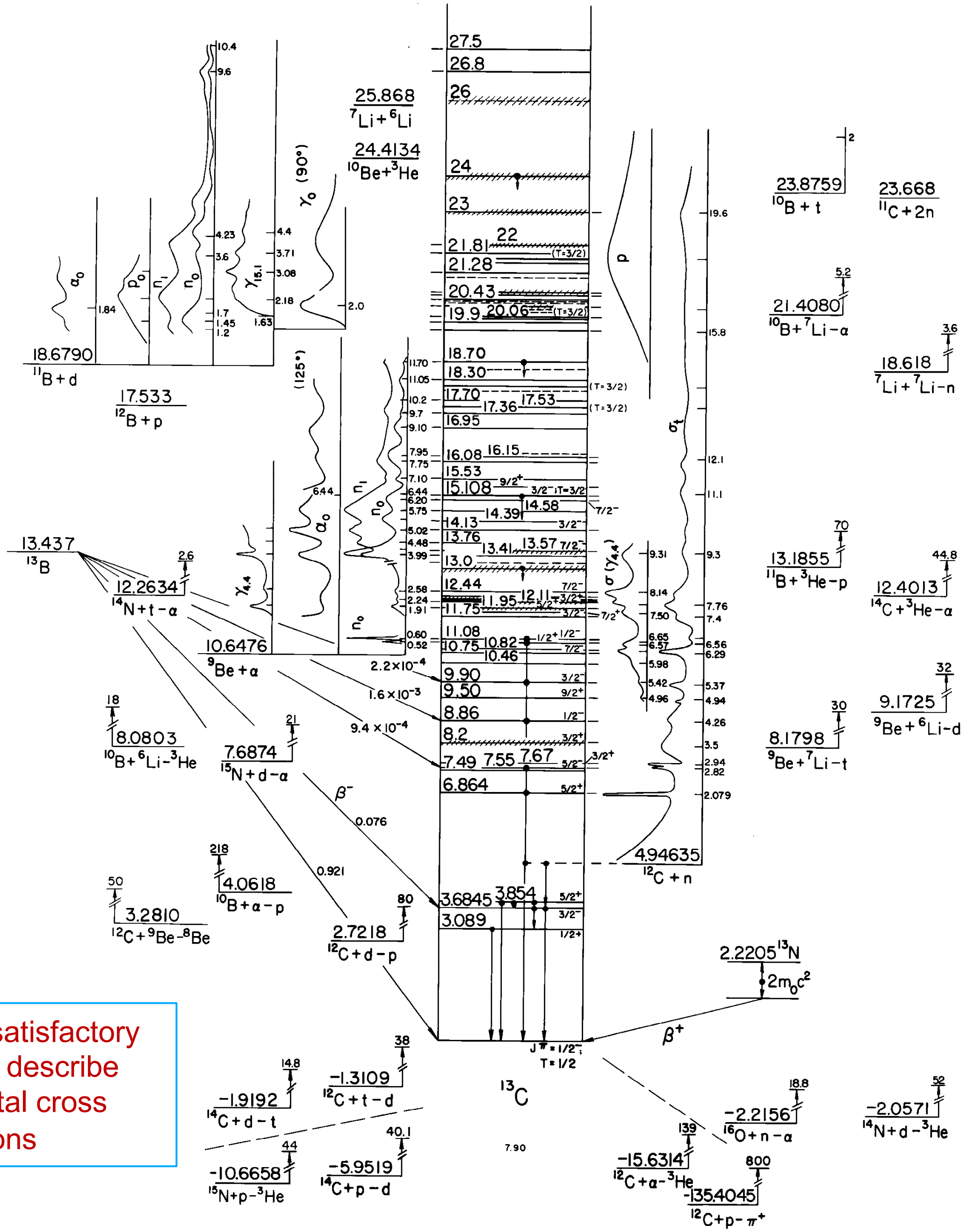
Excitation energies of ^{12}C and ^{12}B as well as the ^{12}B+p threshold adjusted to experiment

^{13}C and ^{12}C(n,p)^{12}B in NCSMC-pheno

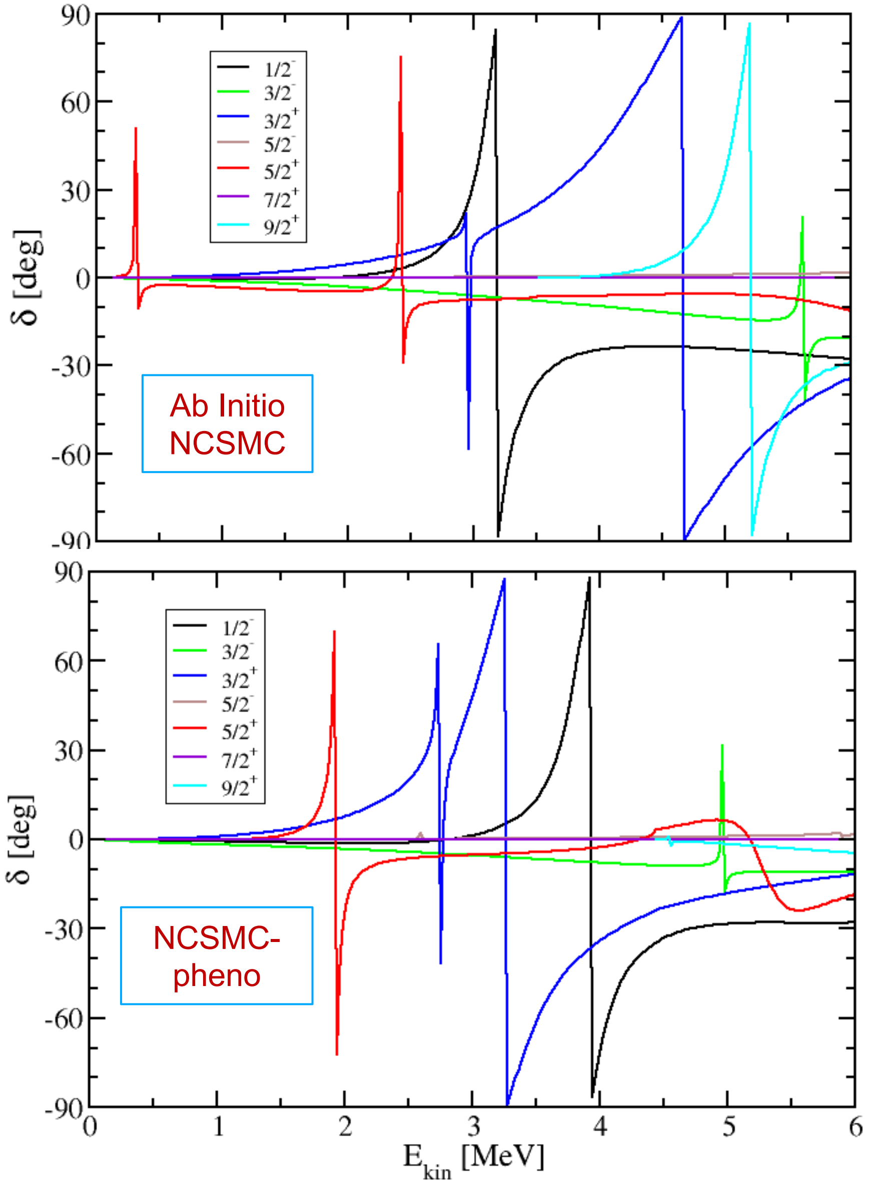
- Input - chiral NN N^{4}LO + 3N$_{lnl}$ interaction – SRG evolved
- NCSMC-pheno results – N_{max}=7
  - Three bound states vs. four in experiment:
    - E(1/2$^-$) = -4.95 MeV vs. Expt. -4.95 MeV
    - E(1/2$^+$)= -1.86 MeV vs. Expt. -1.86 MeV
    - E(3/2$^-$) = -1.26 MeV vs. Expt. -1.26 MeV
    - E(5/2$^+$)= -1.09 MeV vs. Expt. -1.09 MeV
  - Resonances

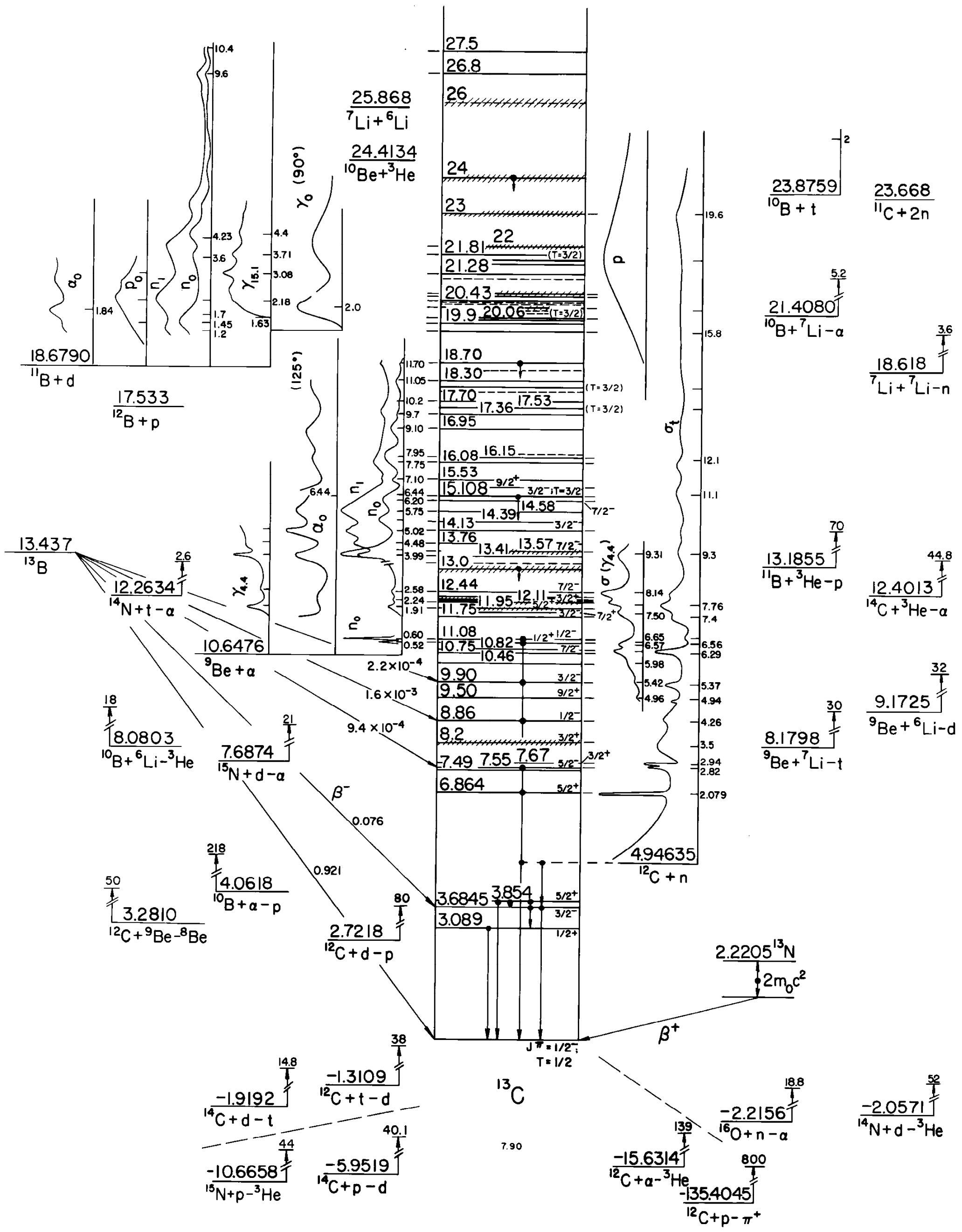


Quantitively satisfactory accuracy to describe experimental cross sections

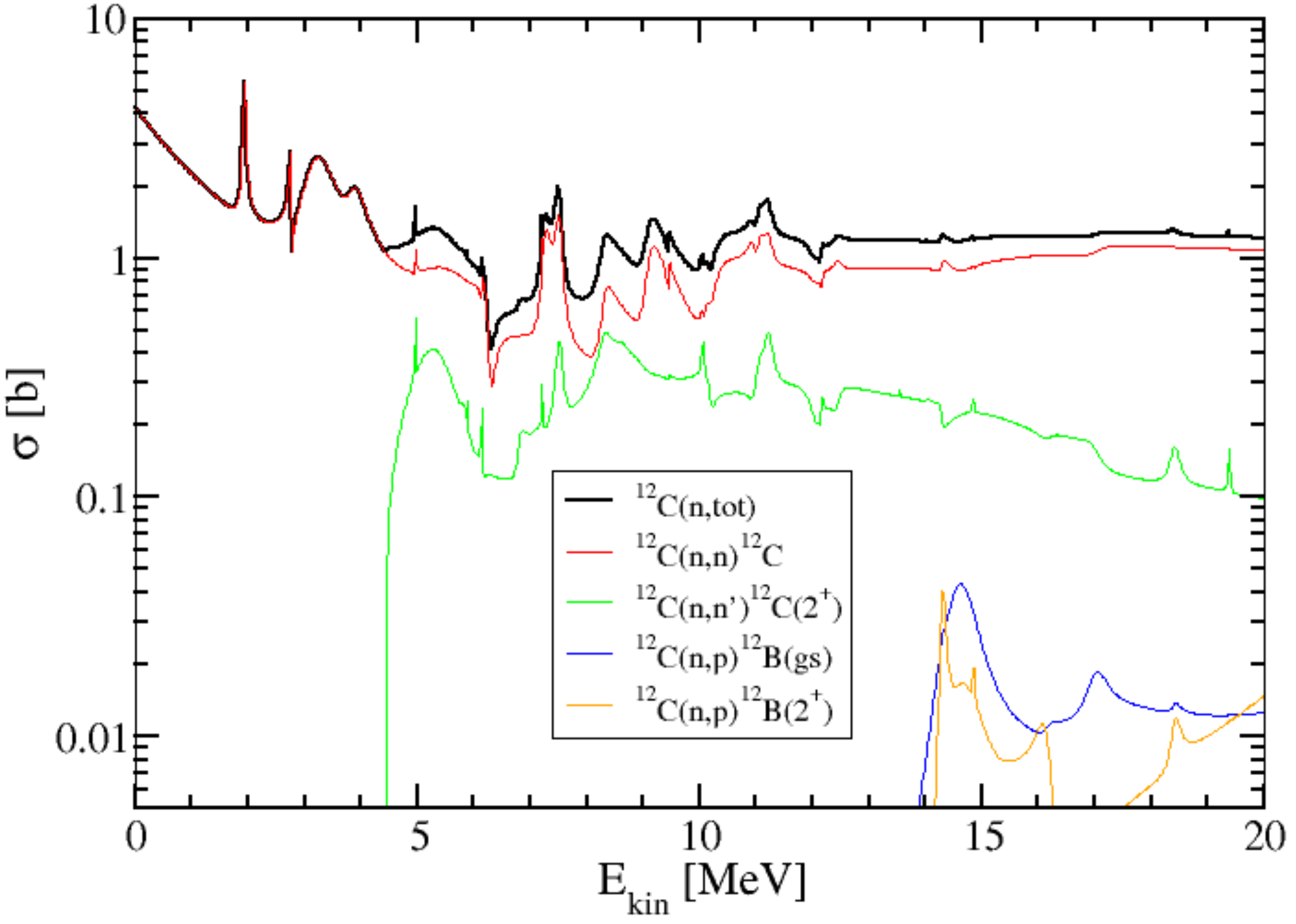


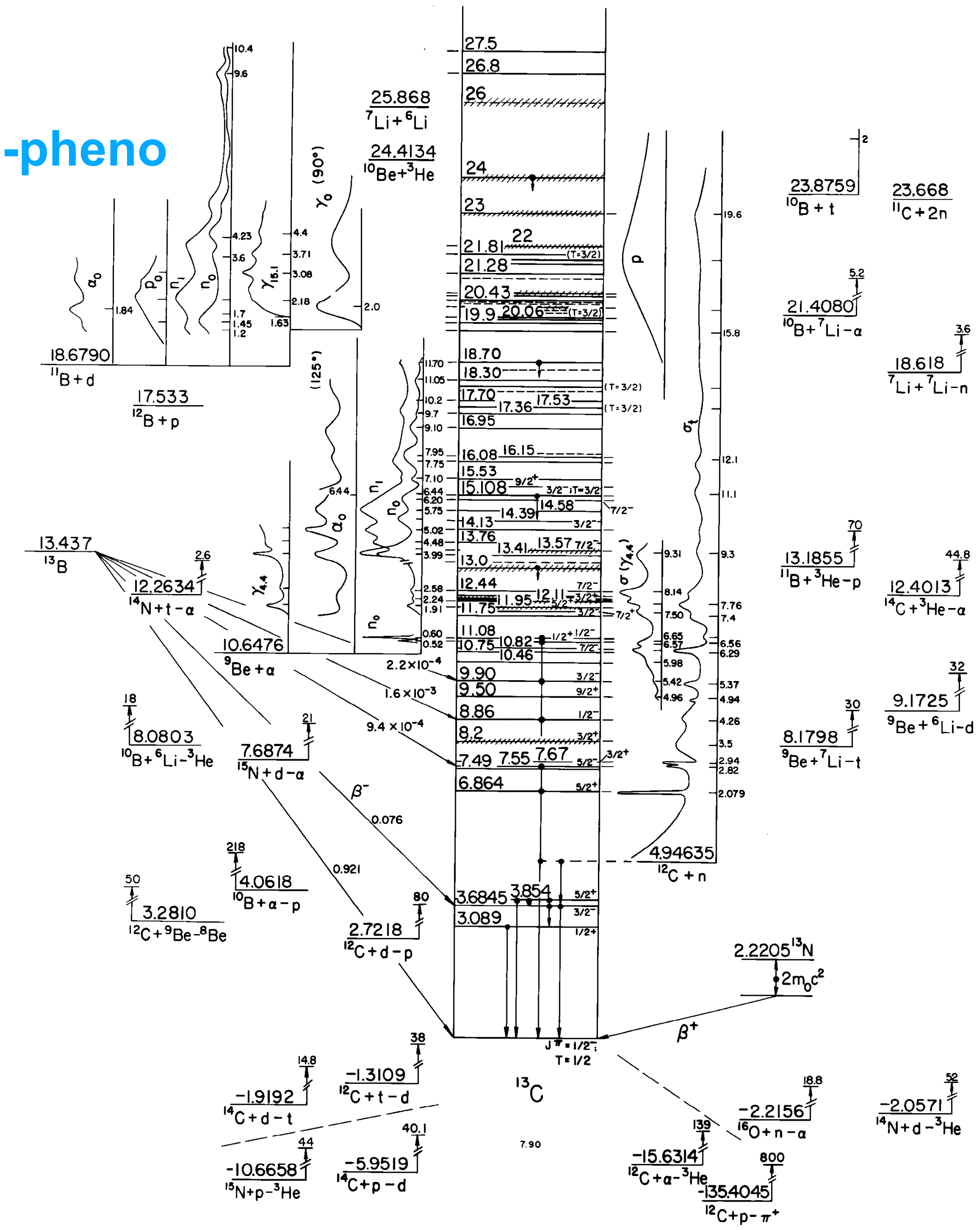
Phase shift comparison



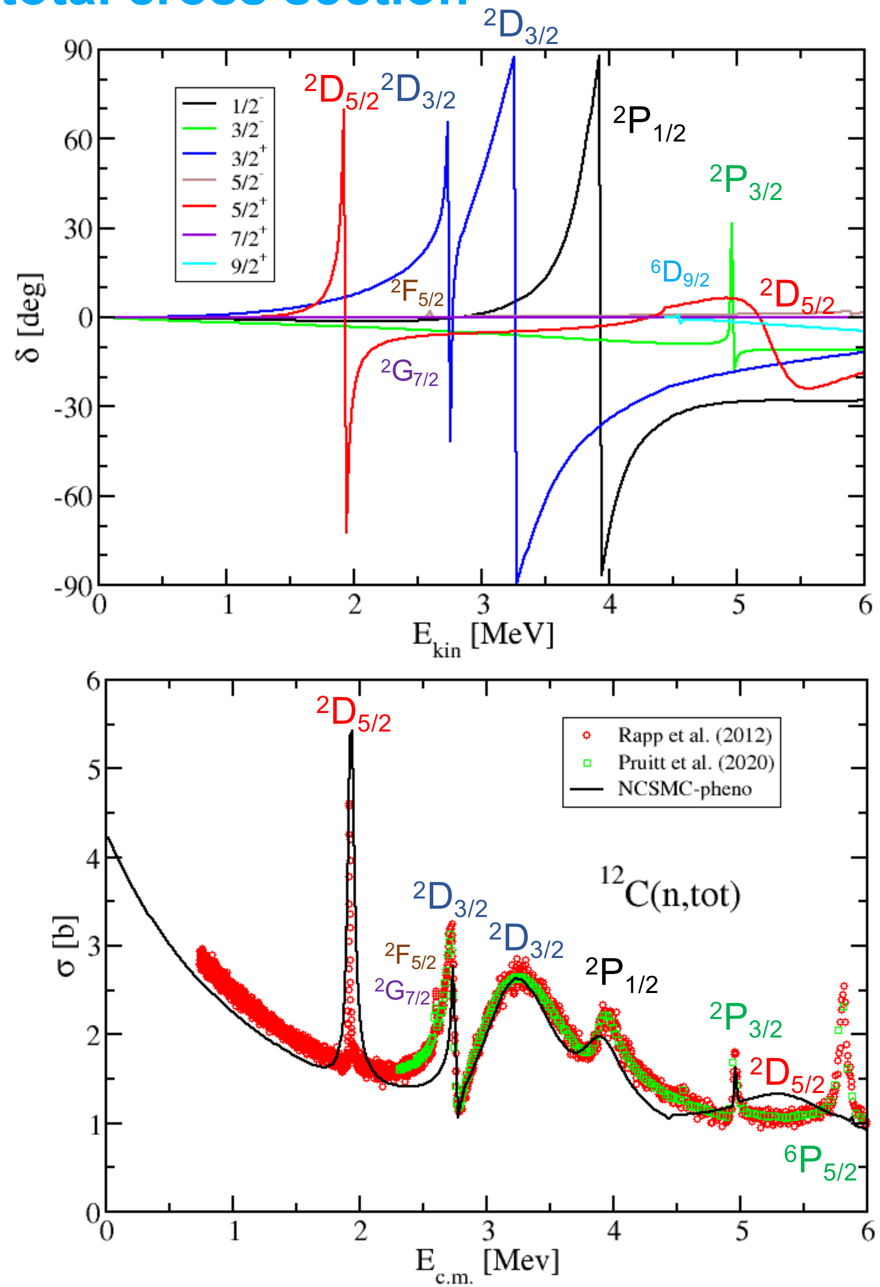


$^{12}C(n,n)^{12}C$ & $^{12}C(n,p)^{12}B$ cross sections in NCSMC-pheno

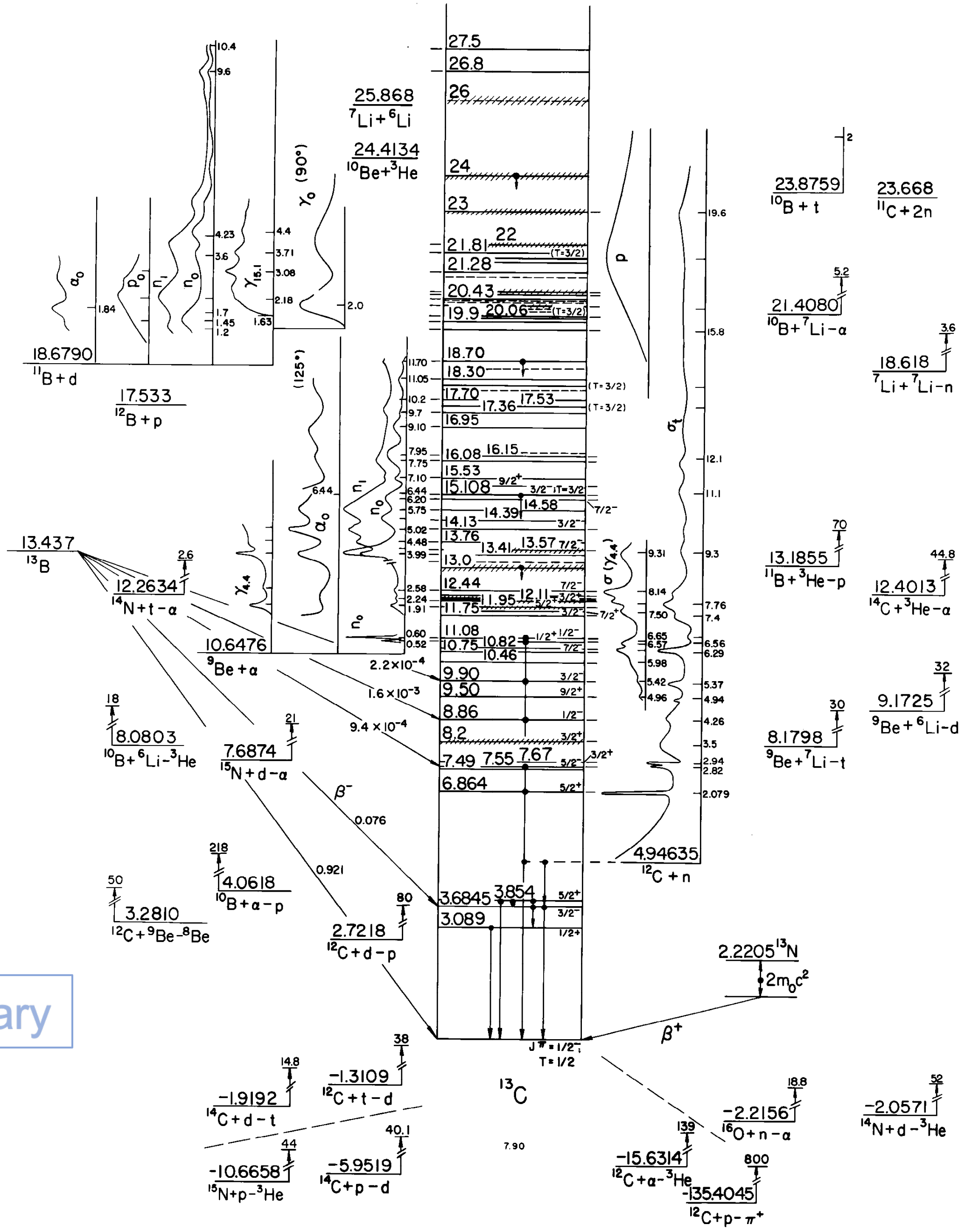




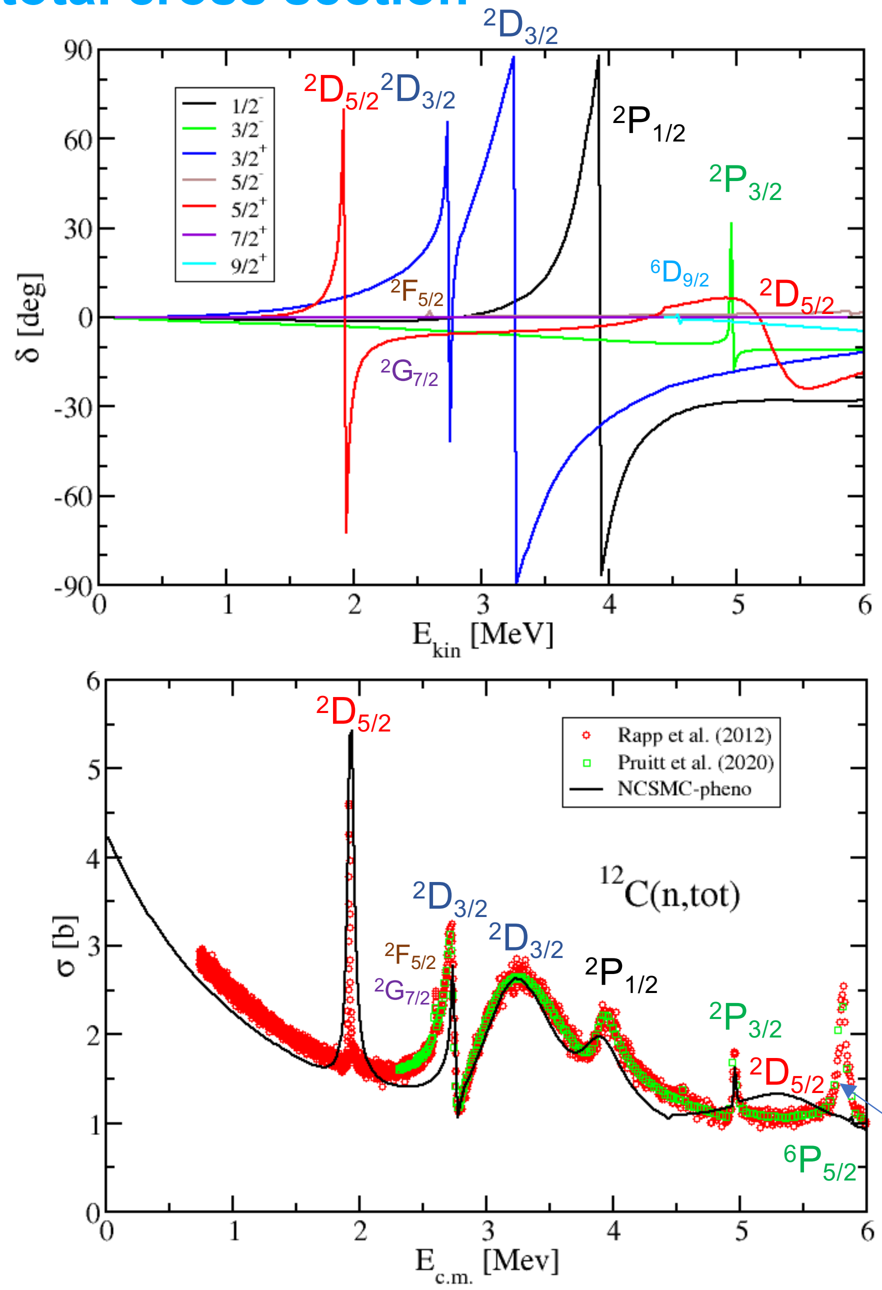
n+^{12}C total cross section



Preliminary

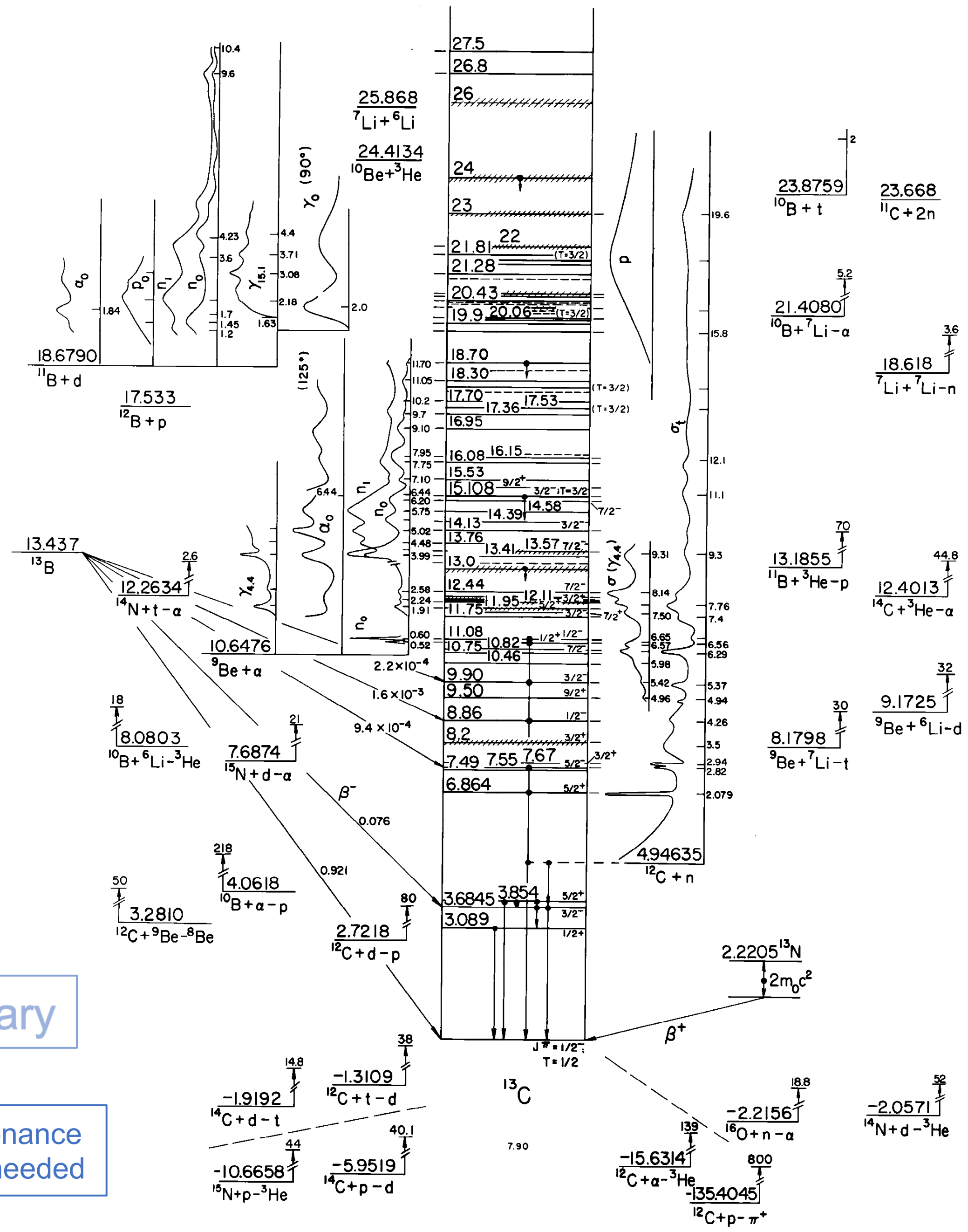


n+^{12}C total cross section

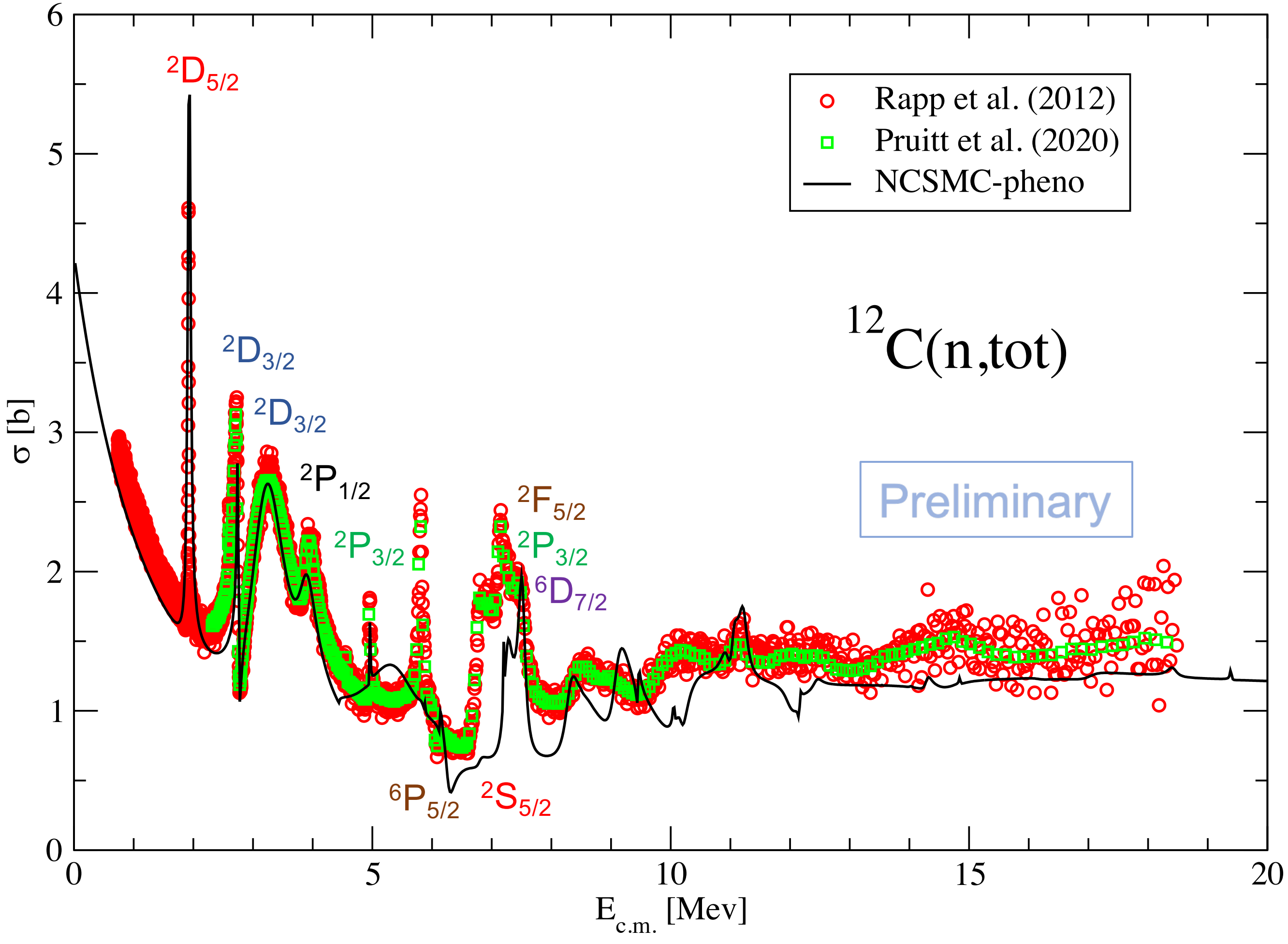


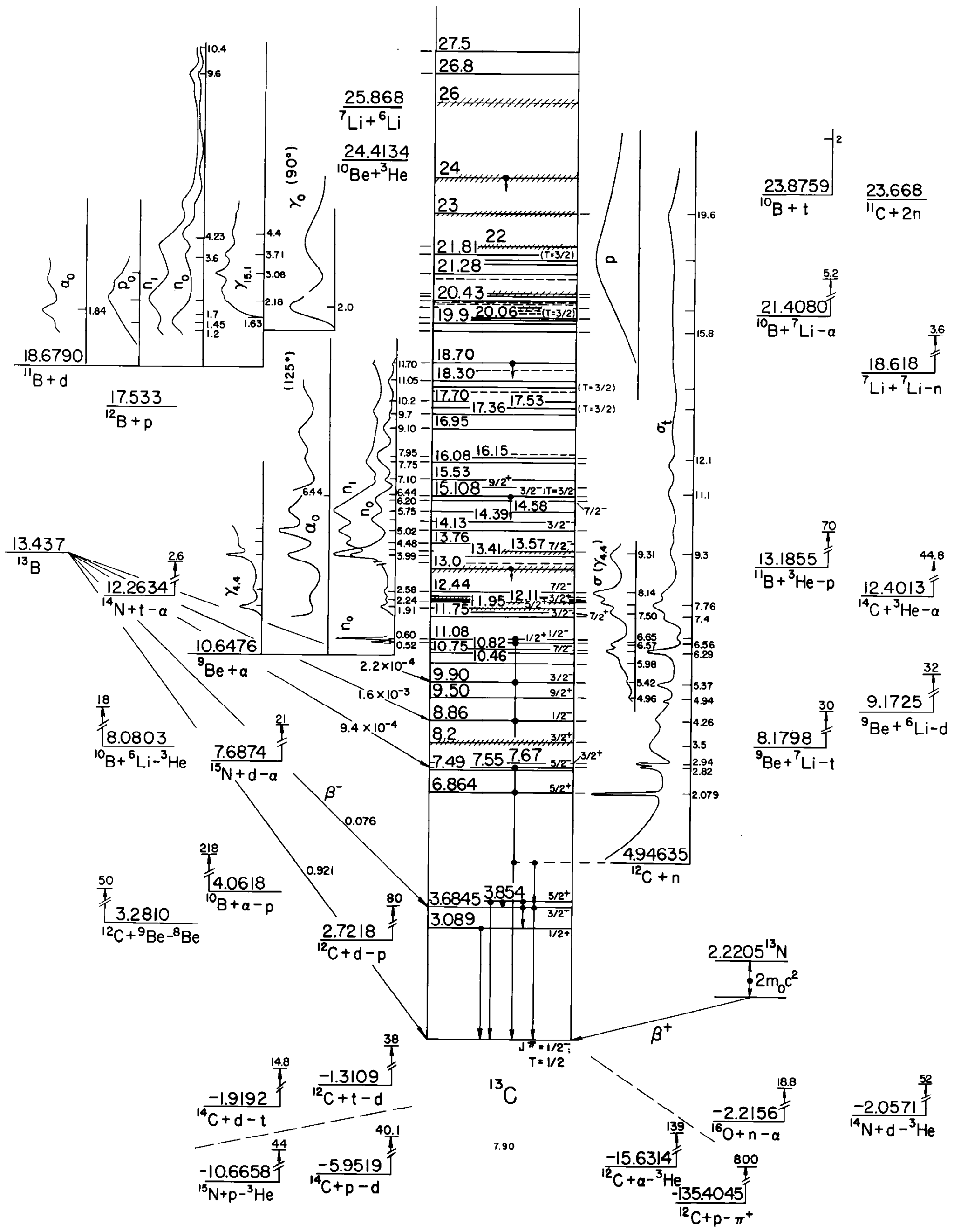
Preliminary

Refined resonance adjustment needed

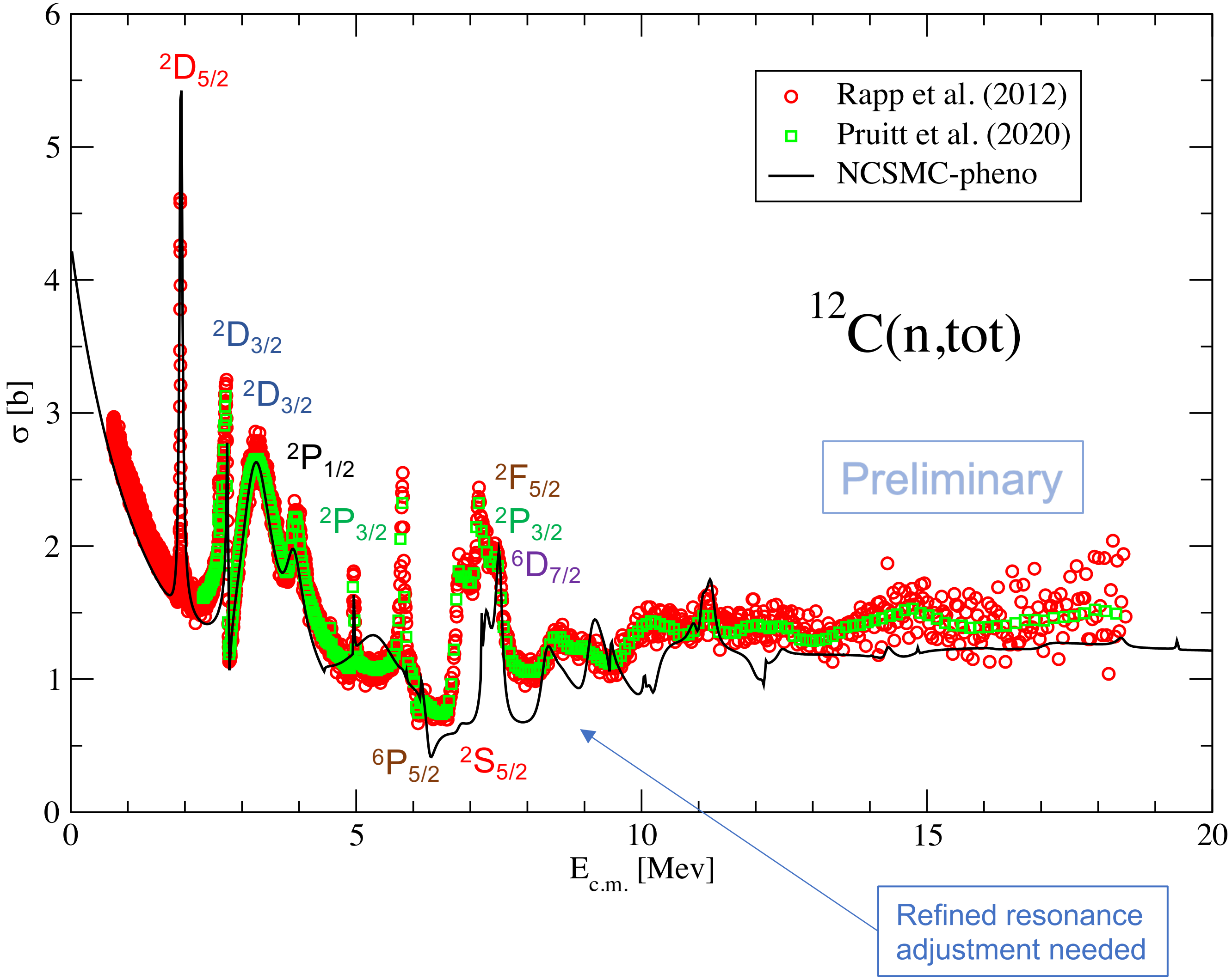


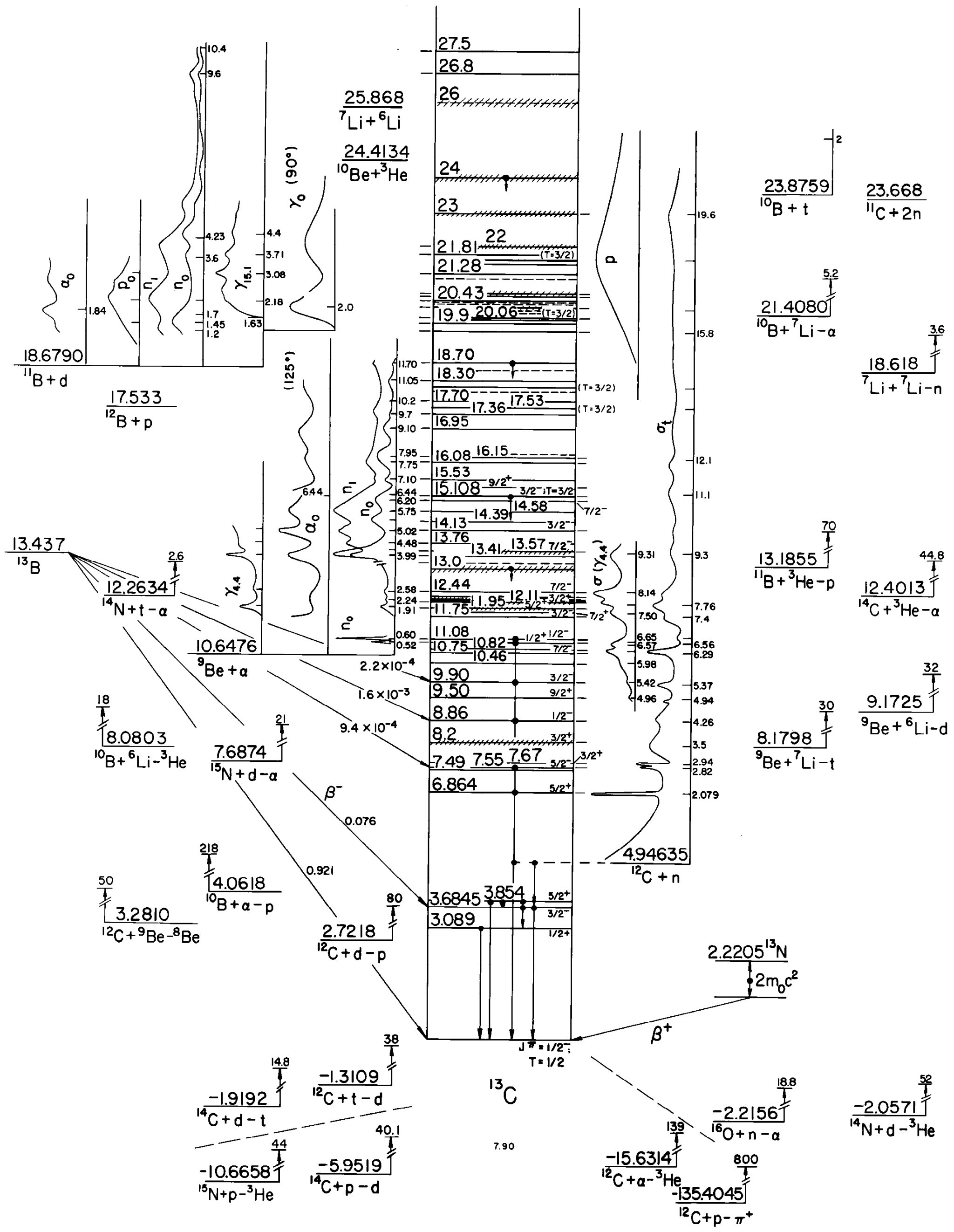
$n+^{12}C$ total cross section



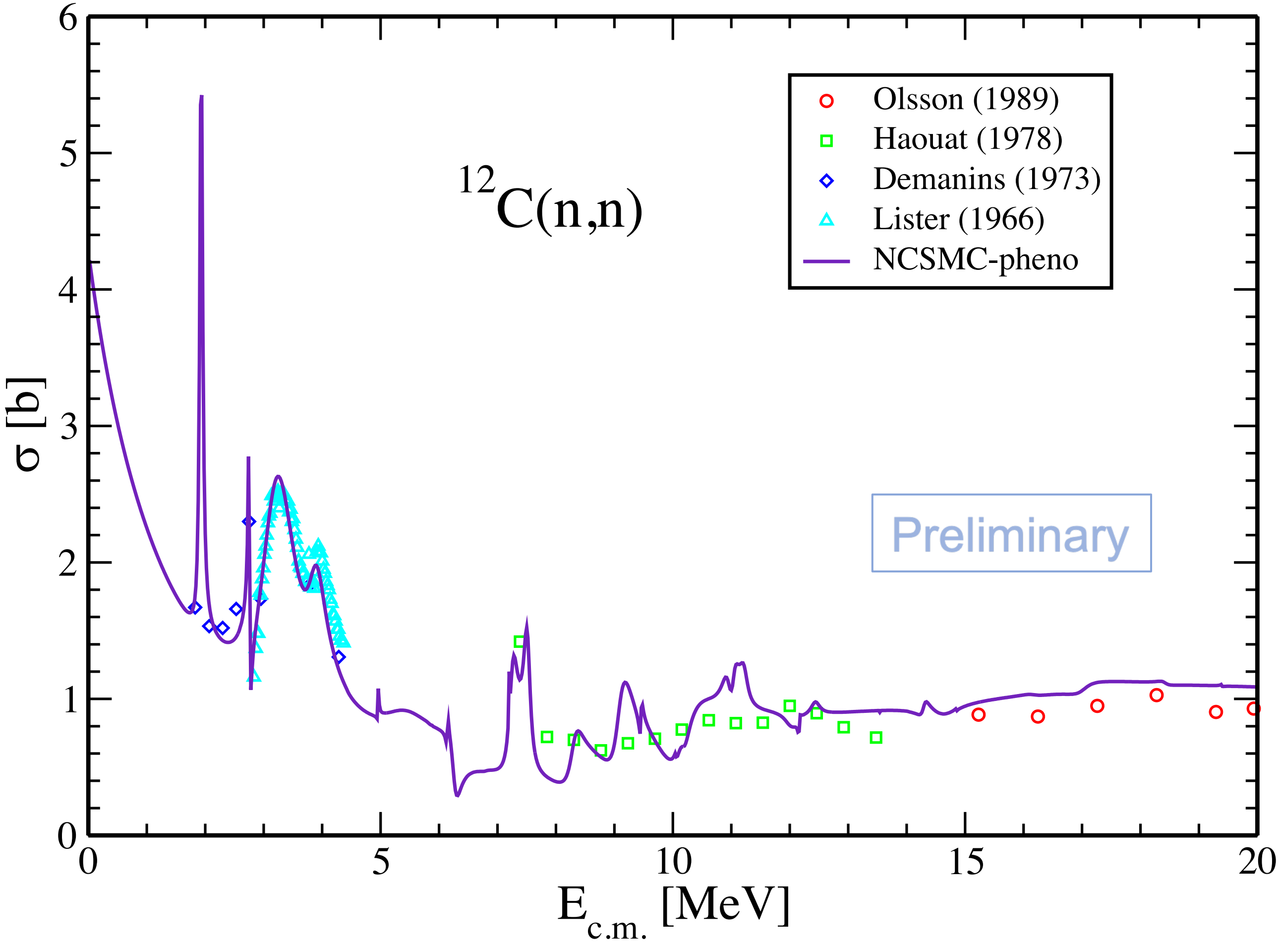


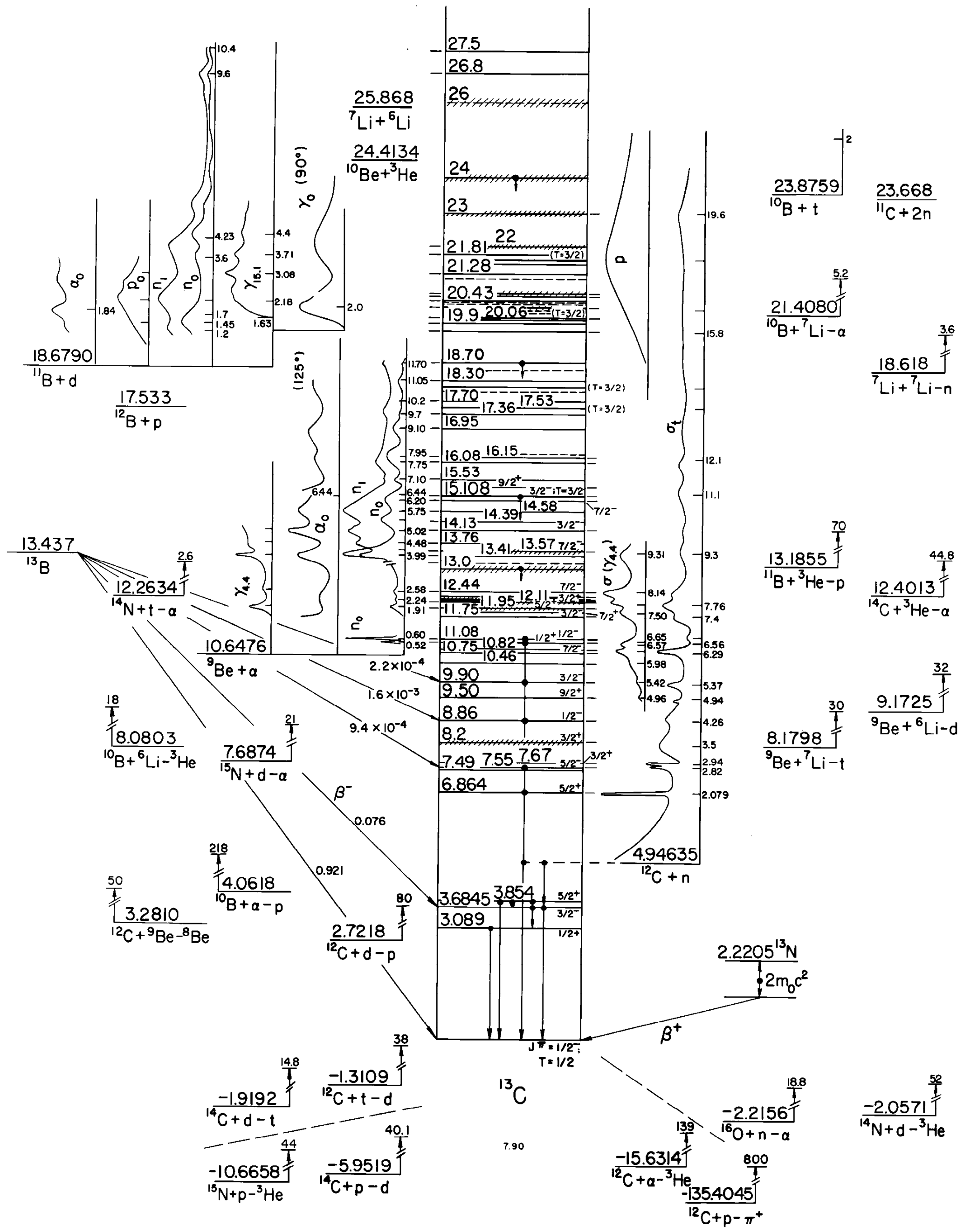
$n+^{12}C$ total cross section



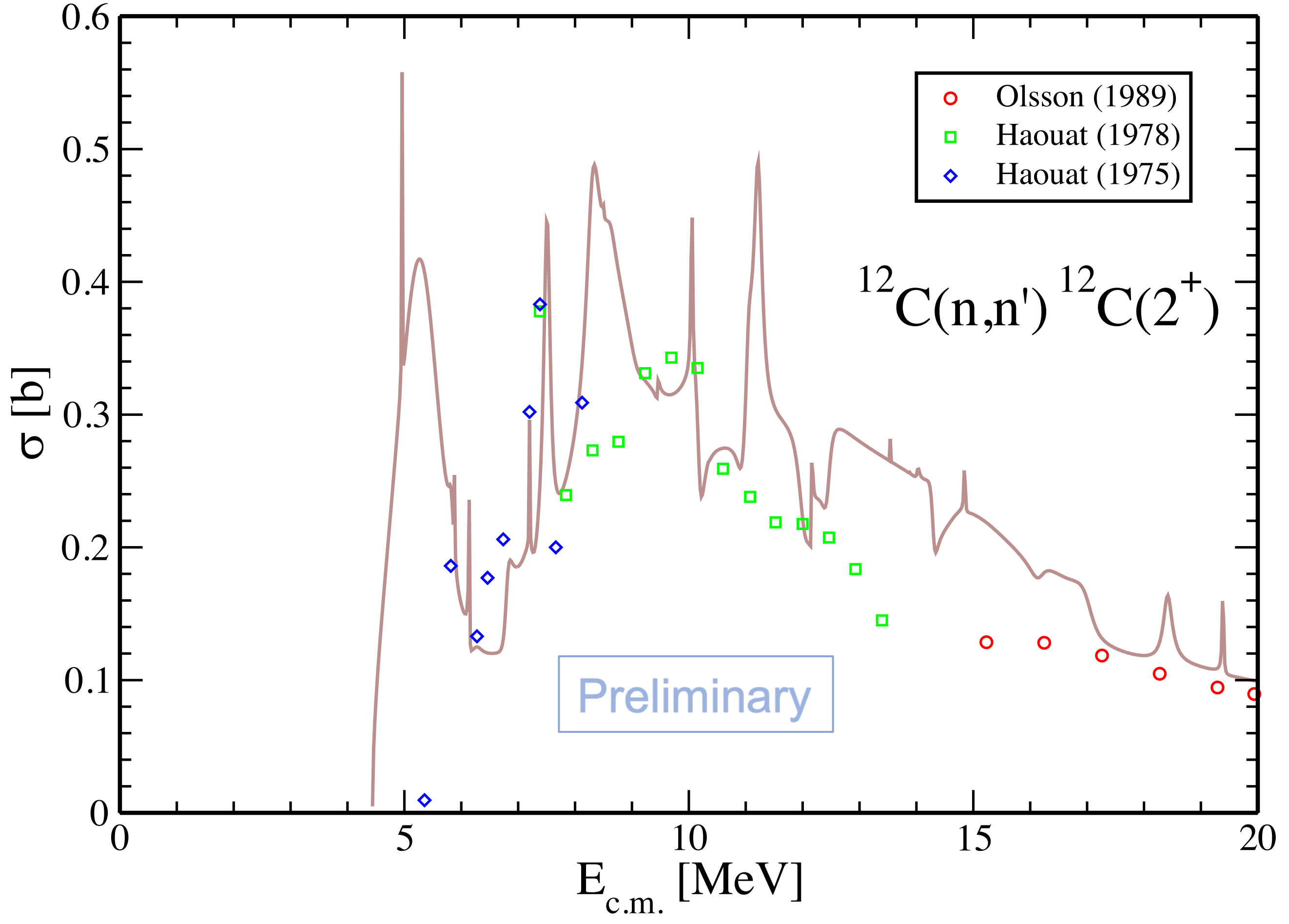


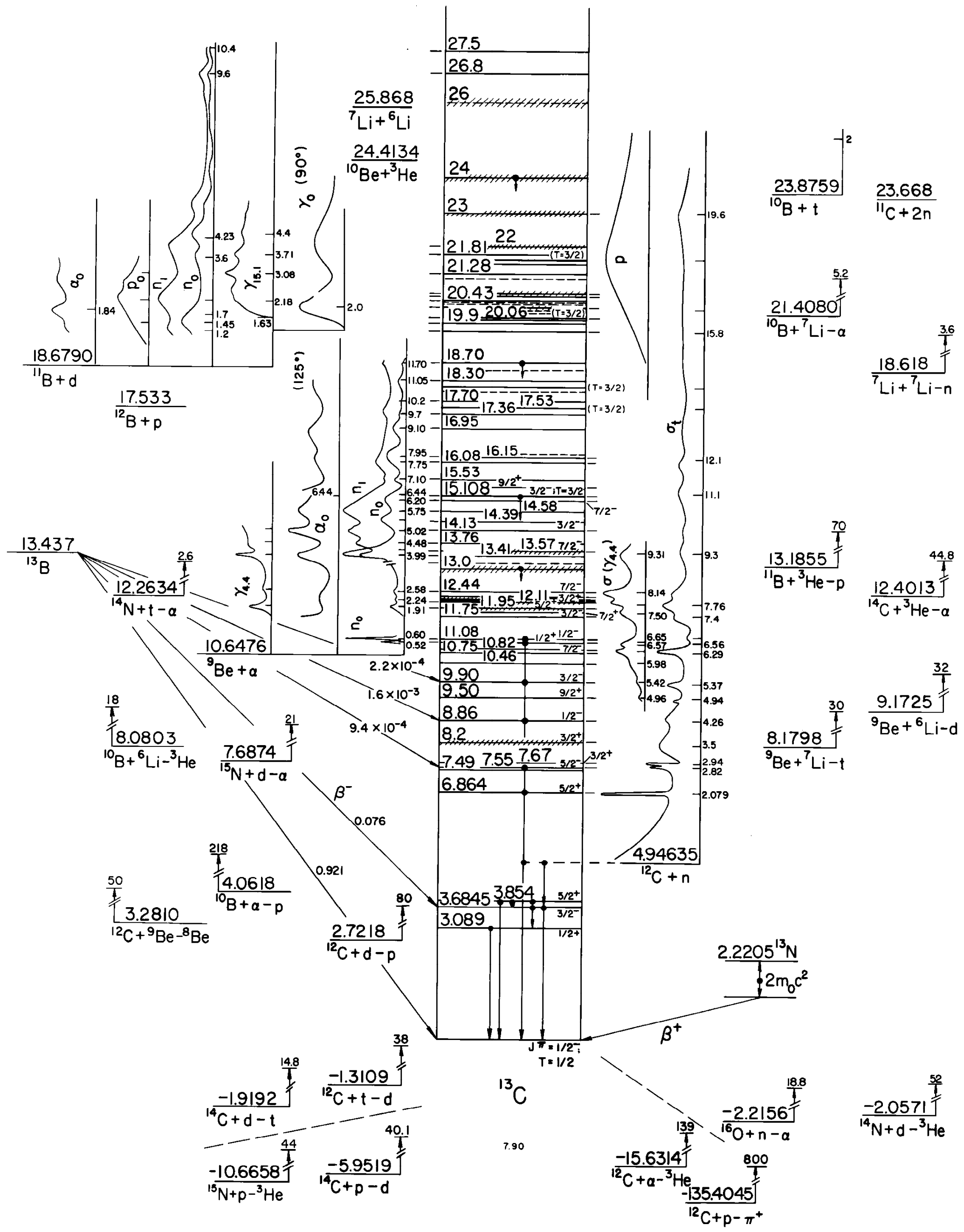
n+^{12}C elastic cross section



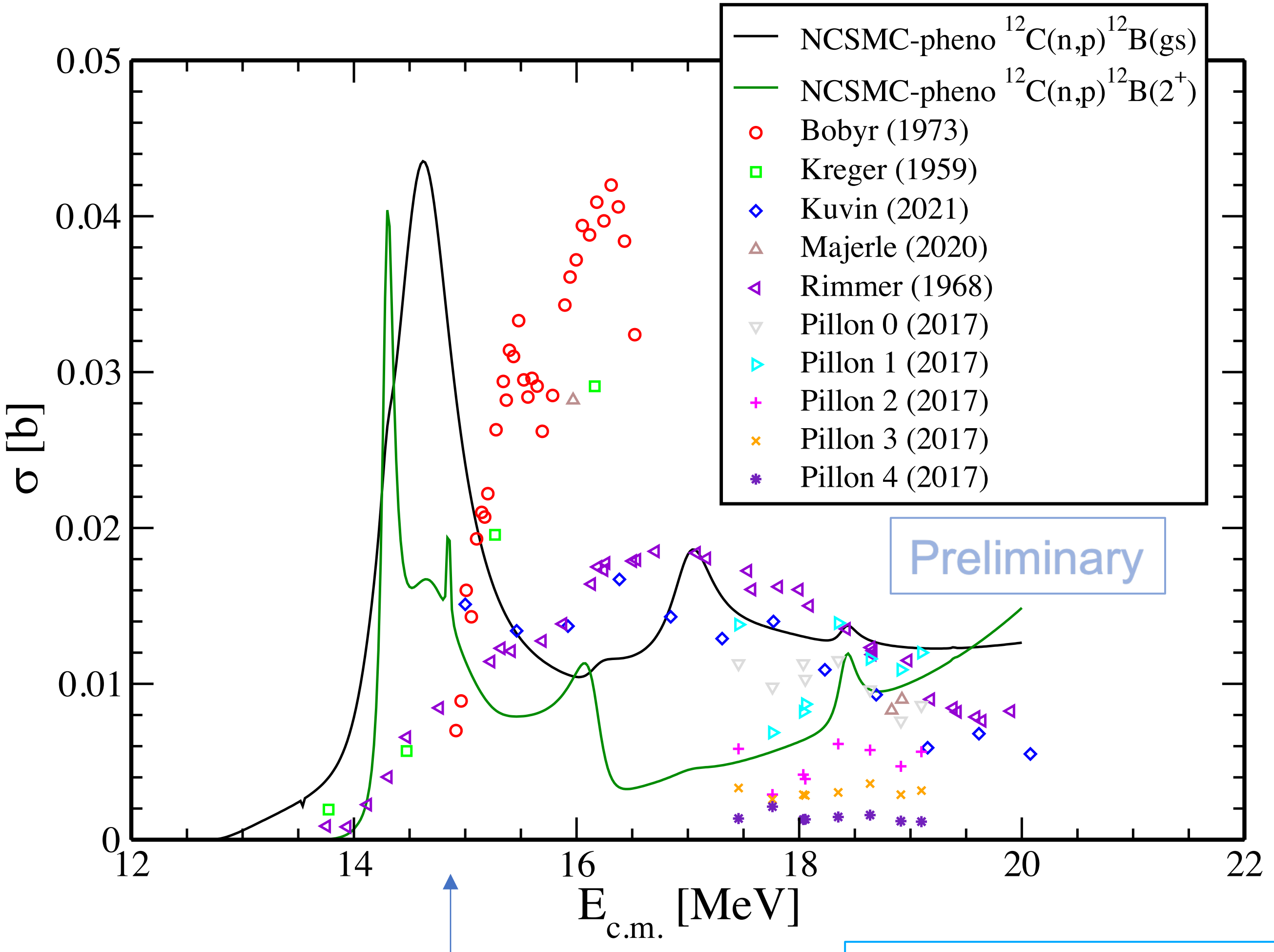


n+^{12}C inelastic cross section

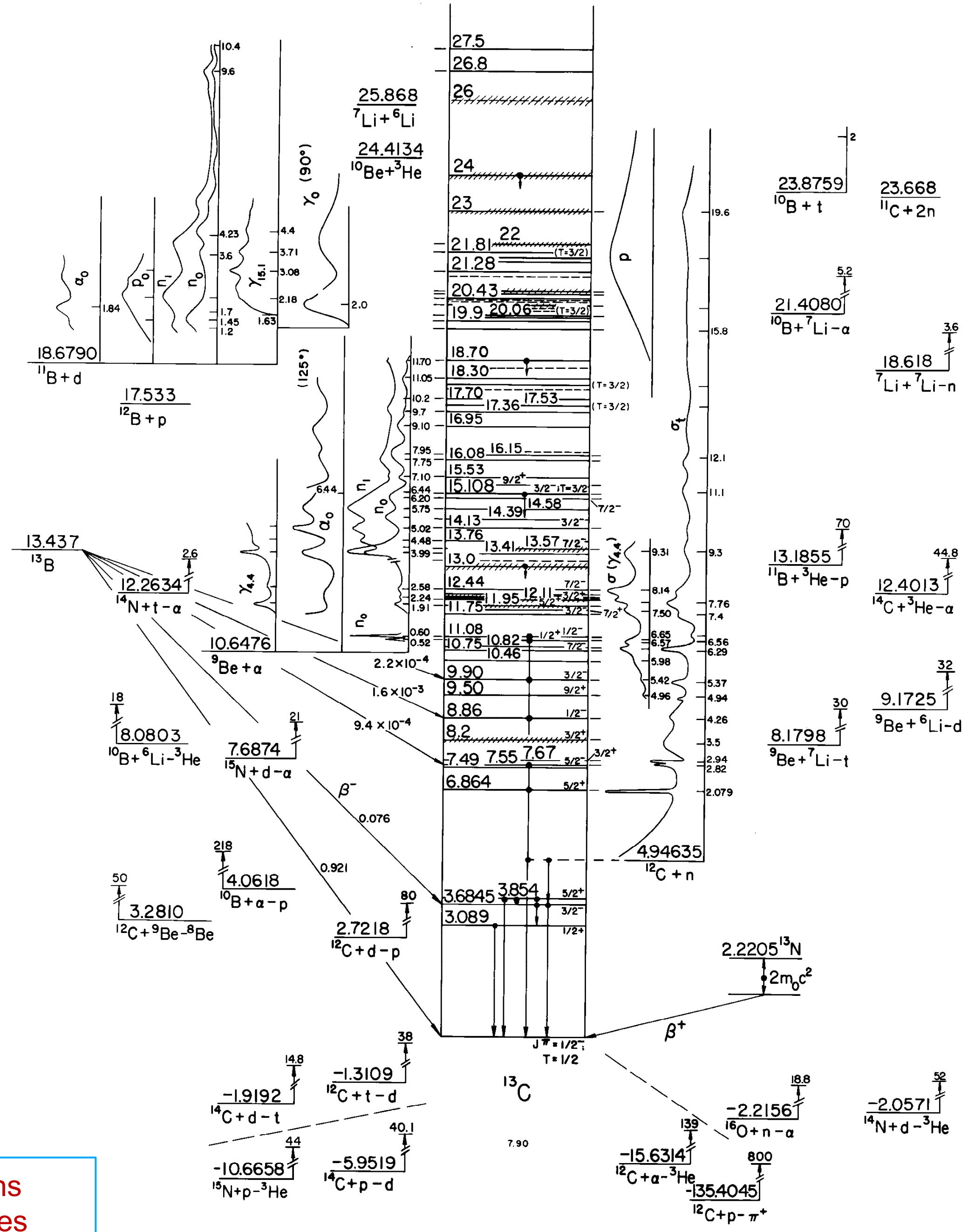




$^{12}C(n,p)^{12}B$ charge-exchange cross section



Resonance adjustment needed



Differential (n,p) cross sections calculated for the two ^{12}B states

Conclusions

- *Ab initio* nuclear theory
  - Makes connections between the low-energy QCD and many-nucleon systems
  - Applicable to nuclear structure, reactions including those relevant for astrophysics, electroweak processes, tests of fundamental symmetries
  - Very recently reach extended to heavy nuclei

- Applications of *ab initio* no-core shell model with continuum to nuclear structure and reactions
  - $^{12}C(n,p)^{12}B$ charge-exchange reaction
    - High density of states in the compound nucleus ^{13}C
      - Regime where typically R-matrix analysis applied
    - Work in progress
      - Fine-tuning the resonance adjustments in the NCSMC-pheno approach
      - More ^{12}B excited states needs to be included

In synergy with experiments, *ab initio* nuclear theory is the right approach to understand low-energy properties of atomic nuclei

TRIUMF

Thank you!
Merci!
Danke!

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Guillaume Hupin (IJCLab)

Discovery, accelerated