# Applications of *ab initio* and phenomenological nuclear reaction theory

Mack C. Atkinson

LLNL-PRES-865739

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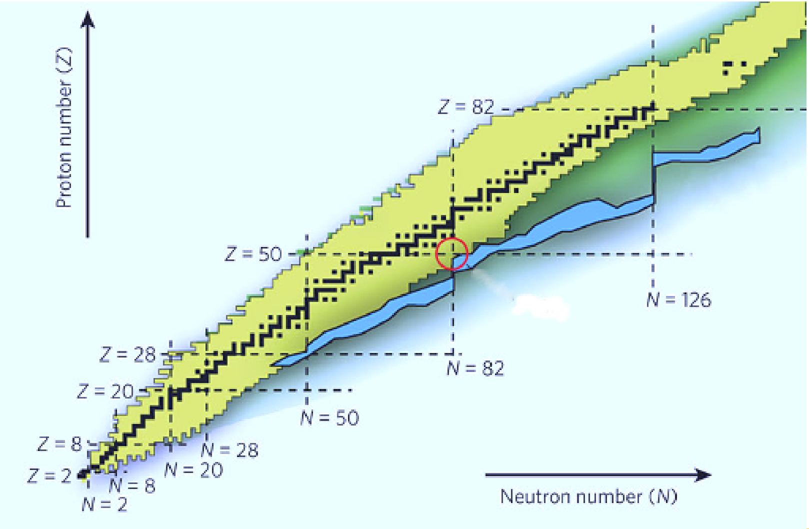
# Nuclear physics is ubiquitous among many fields of science



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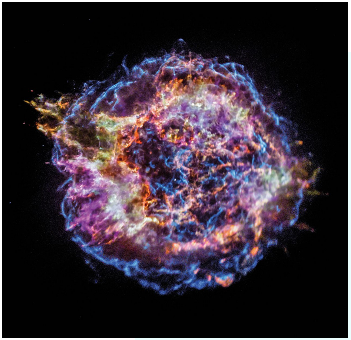

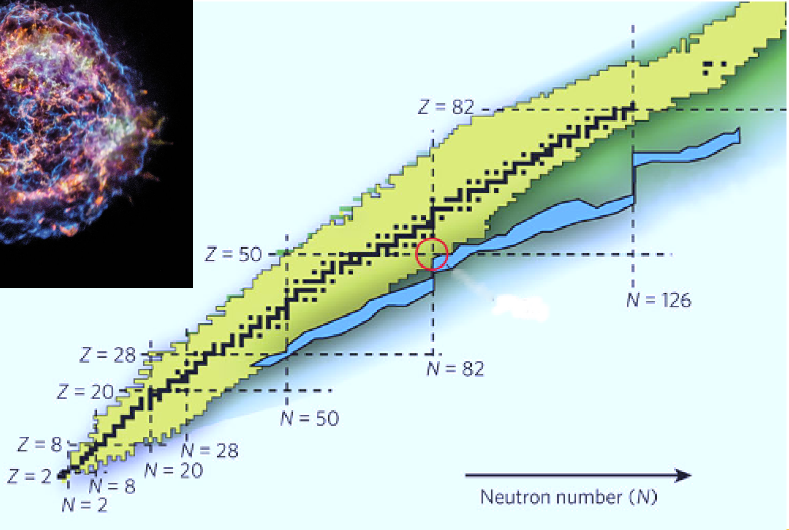

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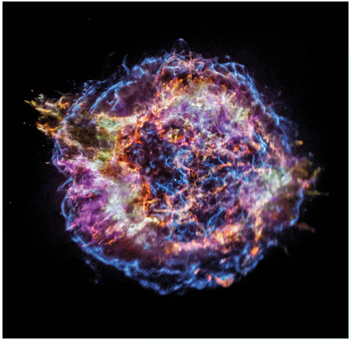

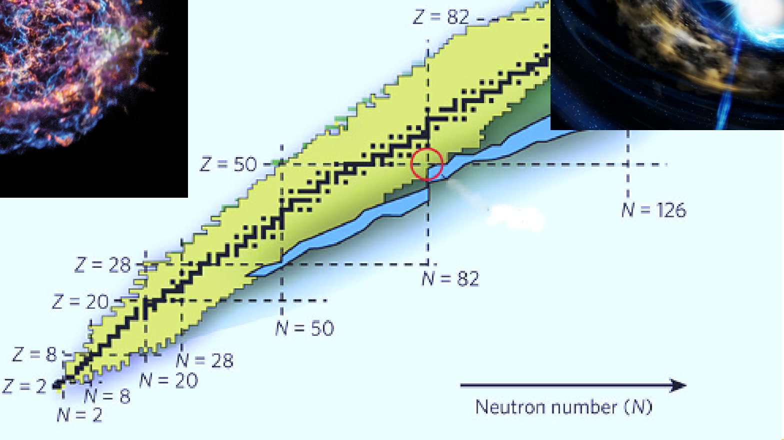


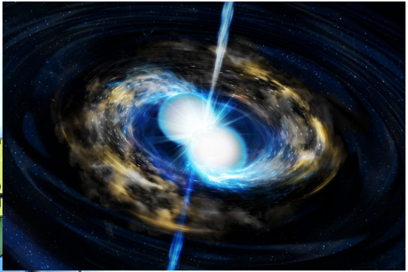

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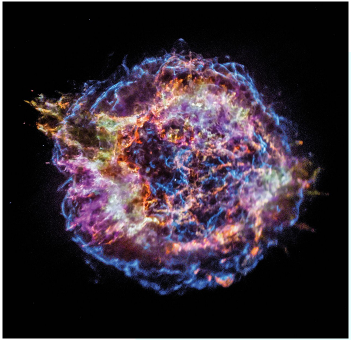

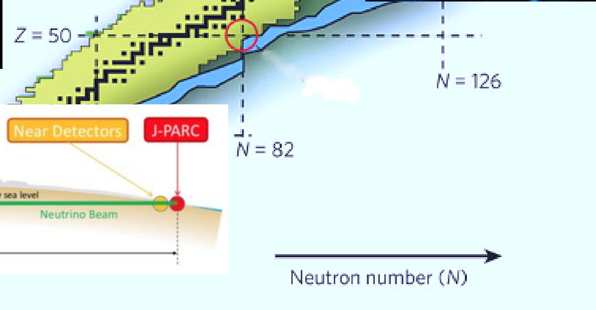


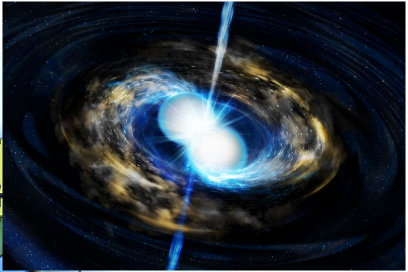

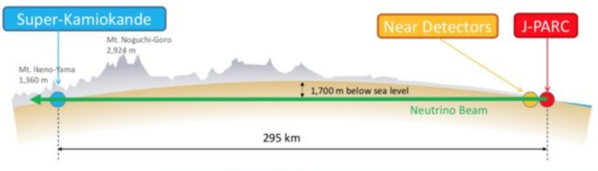

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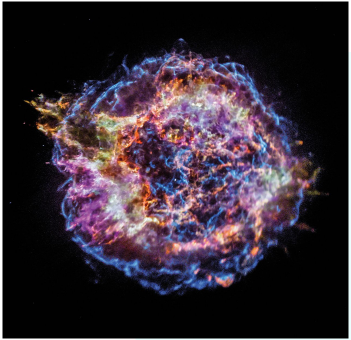

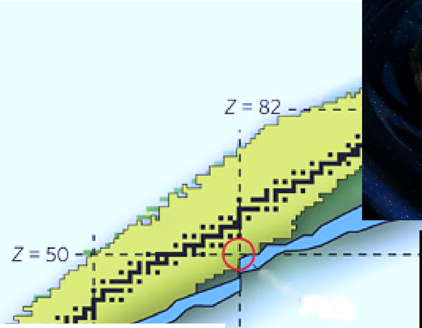


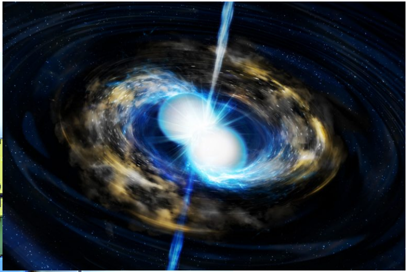

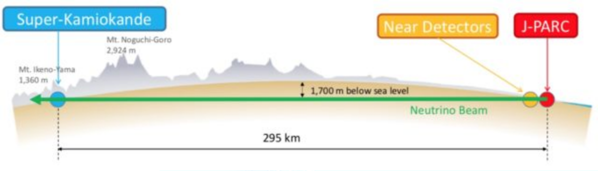


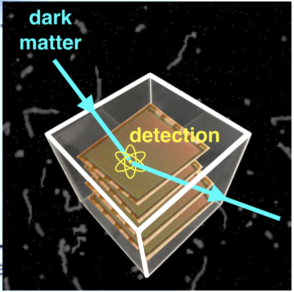

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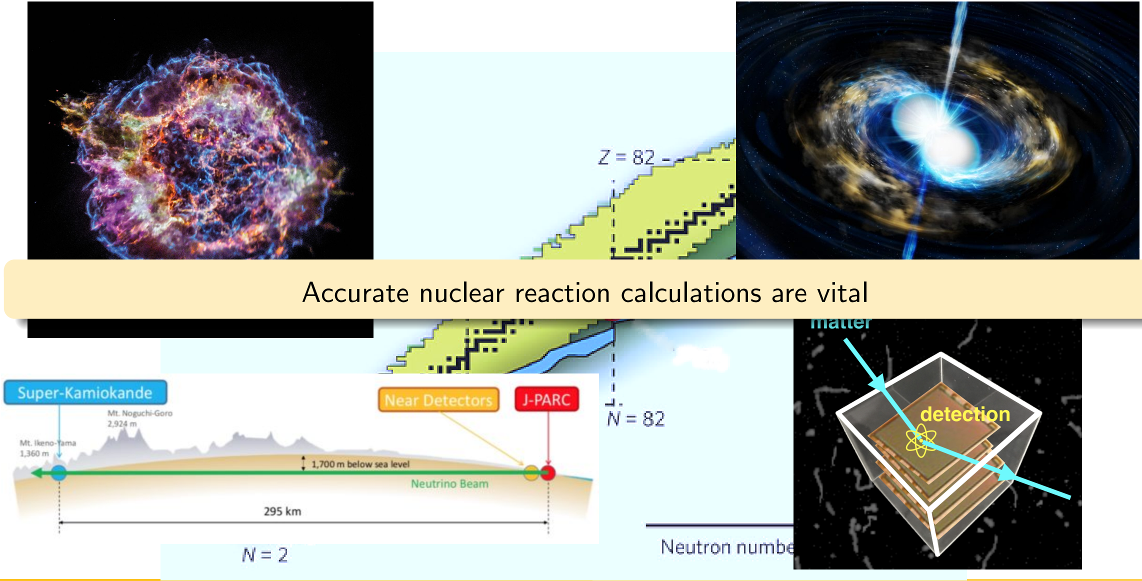
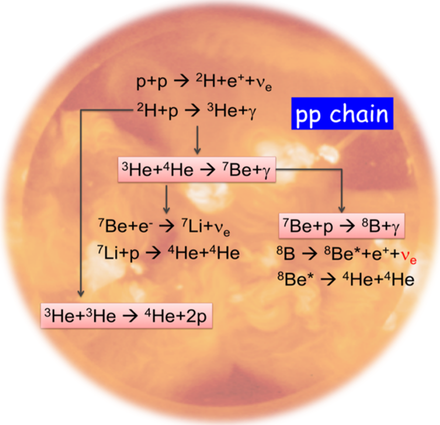



Accurate nuclear reaction calculations are vital

# For example, fusion reactions like $^3$He+$^4$He $\rightarrow$ $^7$Be in our sun



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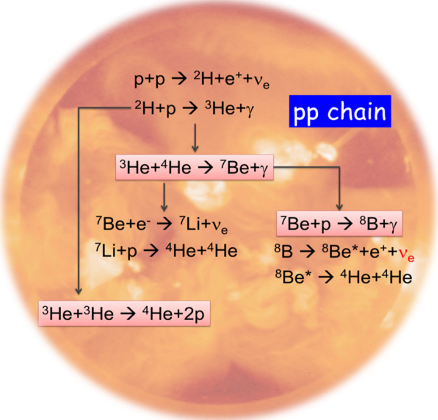


Adelberger *et al.*, Rev Mod Phys **83** 195 (2011)

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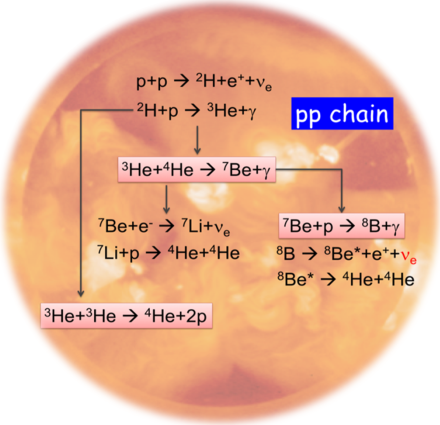


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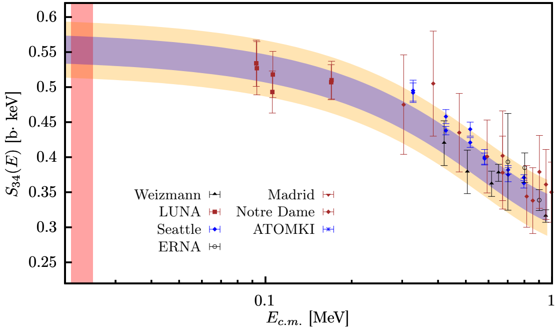


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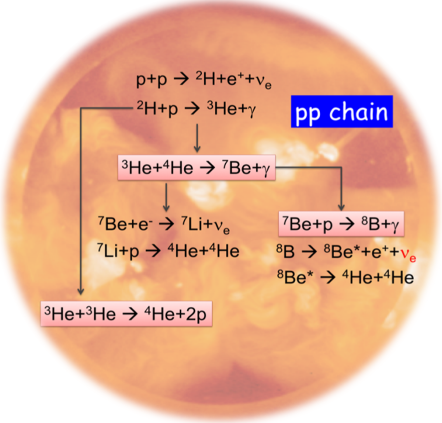

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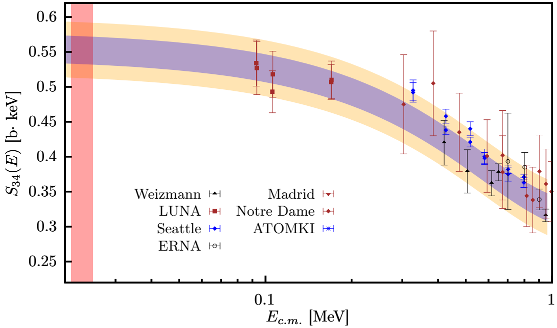


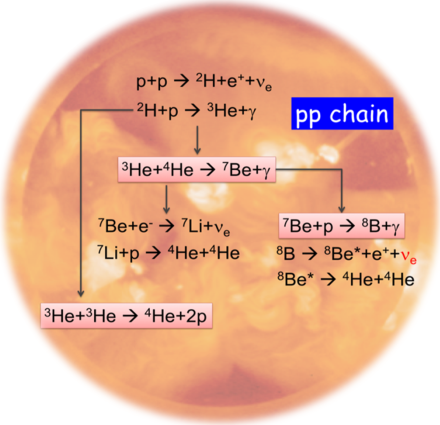


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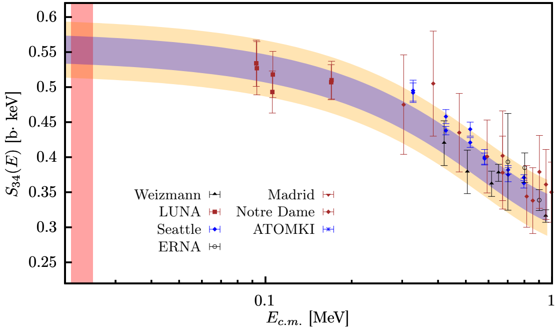
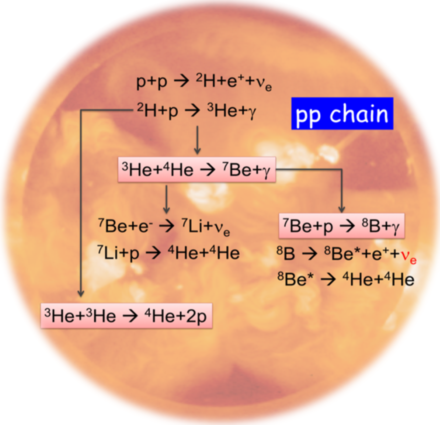
- How to calculate this?

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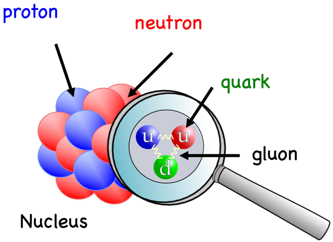
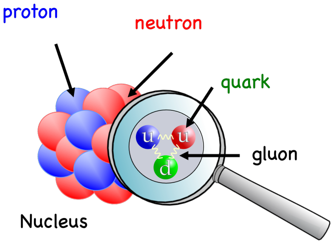
# General picture of the nuclear many-body problem



# General picture of the nuclear many-body problem

$$(T + V)\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_A) = E\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_A)$$



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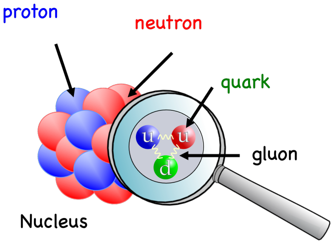


$$V = \frac{1}{2}\sum_{k \neq l = 1}^{A} V_{NN}(\boldsymbol{r}_k, \boldsymbol{r}_l)$$

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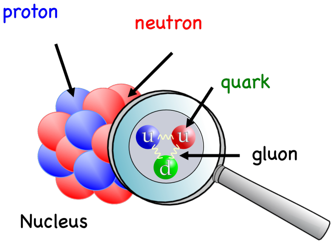


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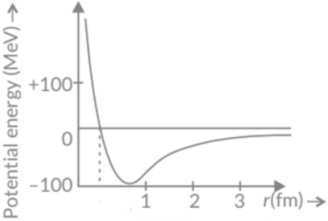

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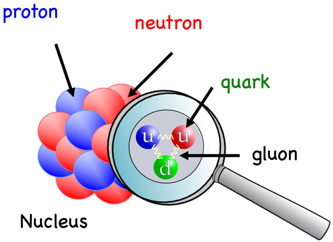


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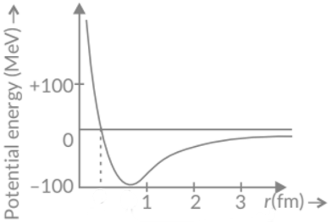

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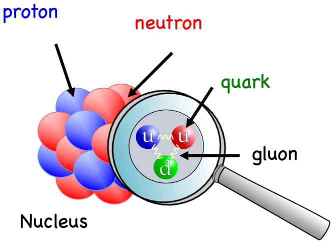


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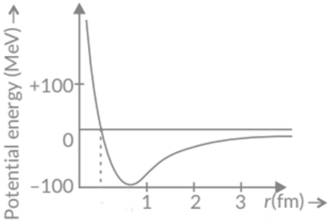


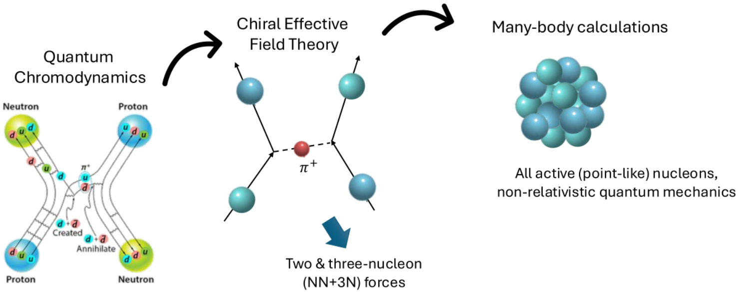

# The *ab initio* method: No-core shell model with continuum (NCSMC)

$$\left\langle \Psi_{bs}\left({}^{7}\mathrm{Be}\right) \middle| \hat{\mathcal{M}}_{\mathrm{EM}} \middle| \Psi_{sc}\left({}^{3}\mathrm{He}+\alpha\right) \right\rangle$$

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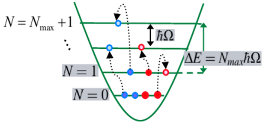


A

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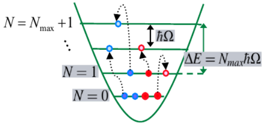



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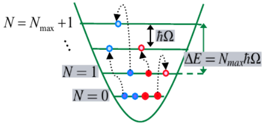


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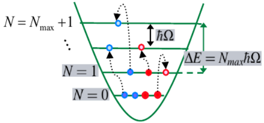



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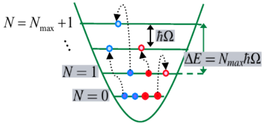


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$\uparrow$

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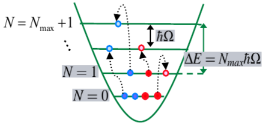



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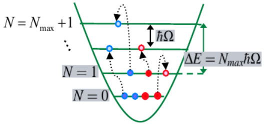



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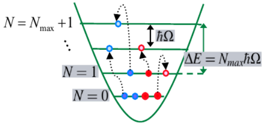


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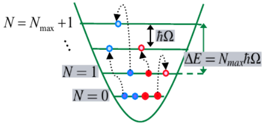


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NCSM

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

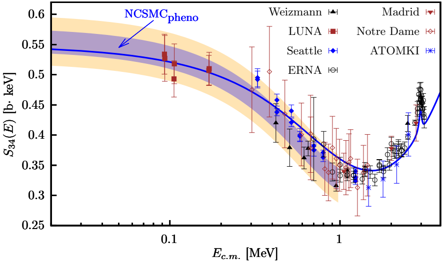
$$|{}^7\mathrm{Be}\rangle \qquad\qquad |\alpha\rangle \otimes |{}^3\mathrm{He}\rangle$$

$$\left\langle \Psi_{bs}\left({}^7\mathrm{Be}\right) \middle| \hat{\mathcal{M}}_{\mathrm{EM}} \middle| \Psi_{sc}\left({}^3\mathrm{He} + \alpha\right) \right\rangle$$

# NCSMC prediction consistent with higher-energy fusion data

M.C. Atkinson *et al.*, PLB **860**, 139189 (2025)

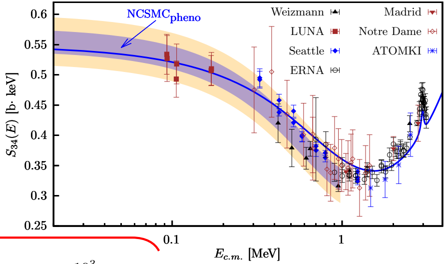
# NCSMC prediction consistent with higher-energy fusion data

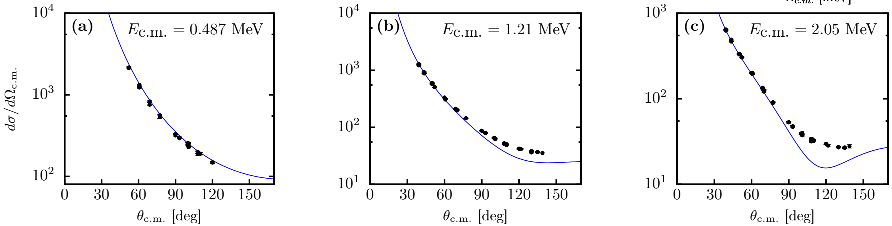



M.C. Atkinson *et al.*, PLB **860**, 139189 (2025)

# NCSMC prediction consistent with higher-energy fusion data

$$\left\langle \Psi_{bs}\left({}^{7}\mathrm{Be}\right) \middle| \hat{\mathcal{M}}_{\mathrm{EM}} \middle| \Psi_{sc}\left({}^{3}\mathrm{He}+\alpha\right) \right\rangle$$



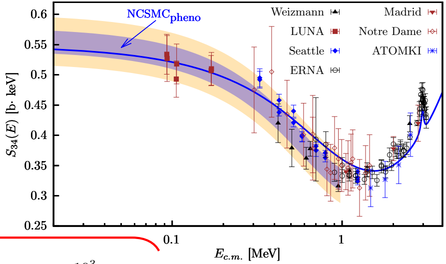



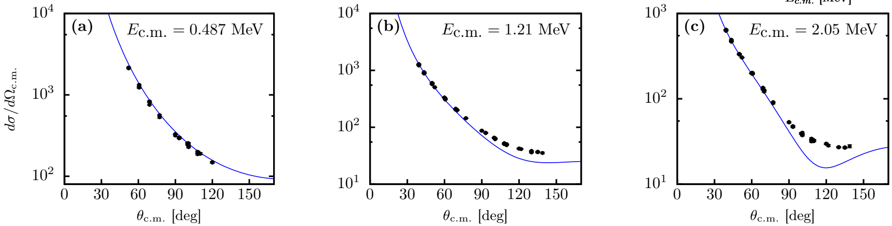

M.C. Atkinson *et al.*, PLB **860**, 139189 (2025)

# NCSMC prediction consistent with higher-energy fusion data

- Elastic-scattering and fusion cross sections should be consistent

$$\left\langle \Psi_{bs}\left({}^{7}\mathrm{Be}\right) \middle| \hat{\mathcal{M}}_{\mathrm{EM}} \middle| \Psi_{sc}\left({}^{3}\mathrm{He}+\alpha\right) \right\rangle$$




M.C. Atkinson *et al.*, PLB **860**, 139189 (2025)

# NCSMC prediction consistent with higher-energy fusion data

- Elastic-scattering and fusion cross sections should be consistent
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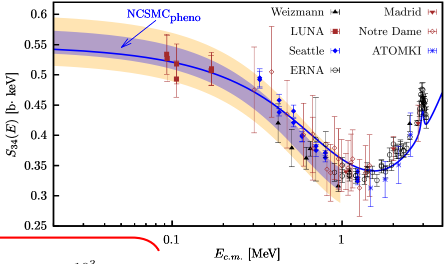
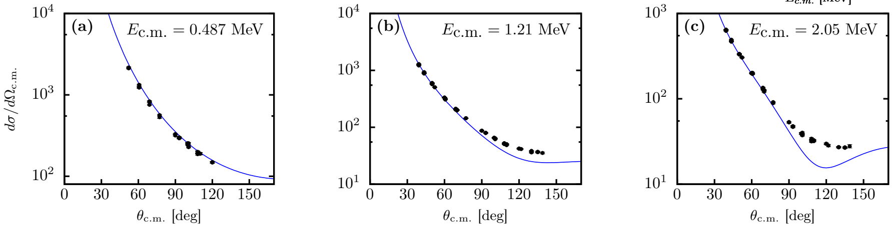
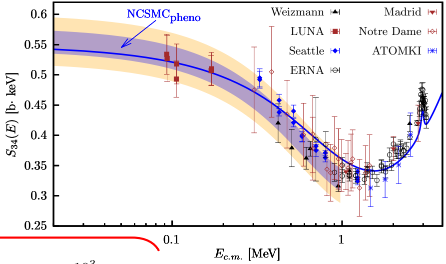


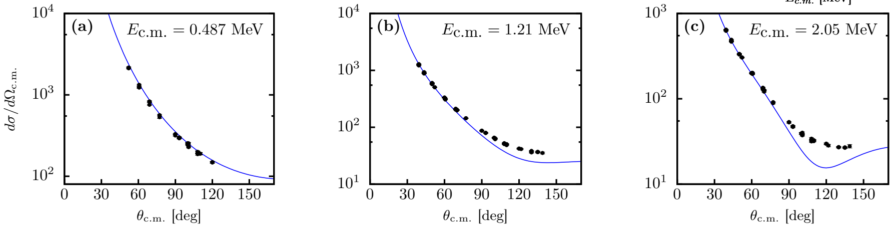

M.C. Atkinson *et al.*, PLB **860**, 139189 (2025)

# NCSMC prediction consistent with higher-energy fusion data

- Elastic-scattering and fusion cross sections should be consistent
- Missing ${}^6$Li+$p$?
- Could also point to unconstrained aspects of $V_{NN}$

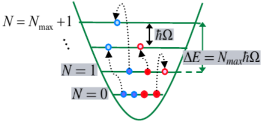



$$\left\langle \Psi_{bs}\left({}^7\mathrm{Be}\right) \middle| \hat{\mathcal{M}}_{\mathrm{EM}} \middle| \Psi_{sc}\left({}^3\mathrm{He}+\alpha\right) \right\rangle$$



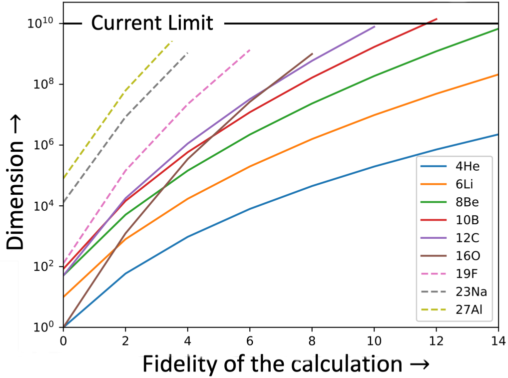

M.C. Atkinson *et al.*, PLB **860**, 139189 (2025)

# NCSMC method is intractable for larger nuclei – how to proceed?





$$\Psi^A = \sum_{N=0}^{N_{max}} \sum_i c_{Ni} \Phi_{Ni}^A$$



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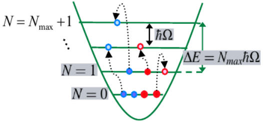



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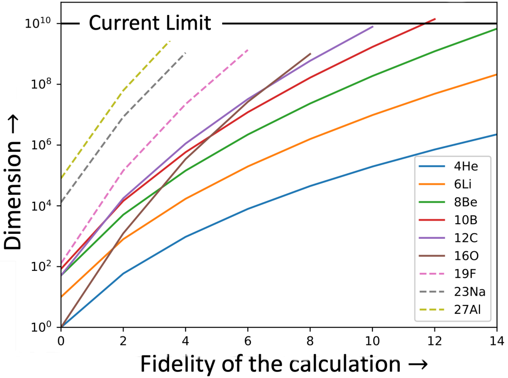


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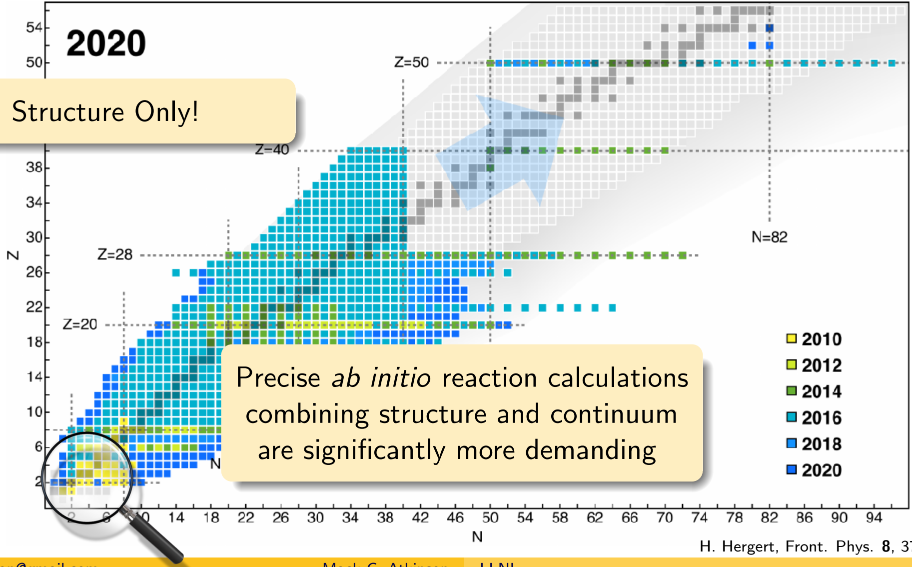
Scaling even worse for full NCSMC

# NCSMC method is intractable for larger nuclei – how to proceed?

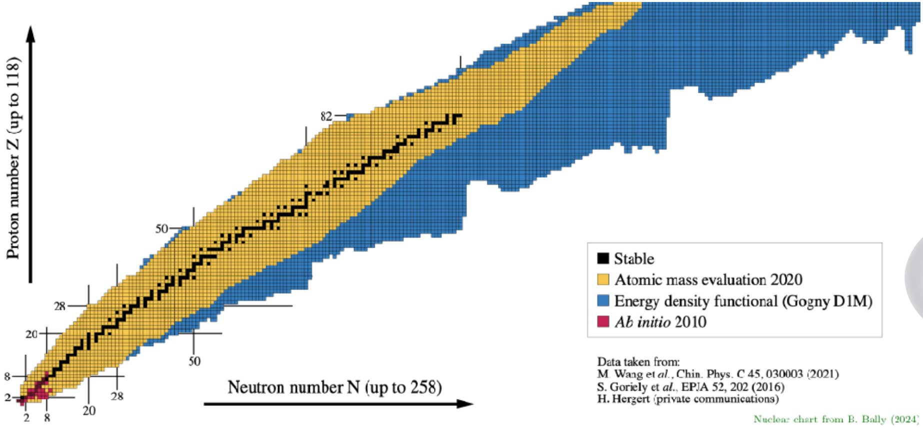


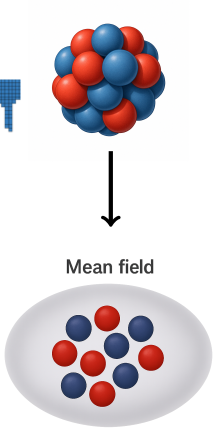

Structure Only!

Precise *ab initio* reaction calculations combining structure and continuum are significantly more demanding

H. Hergert, Front. Phys. **8**, 379 (2020)

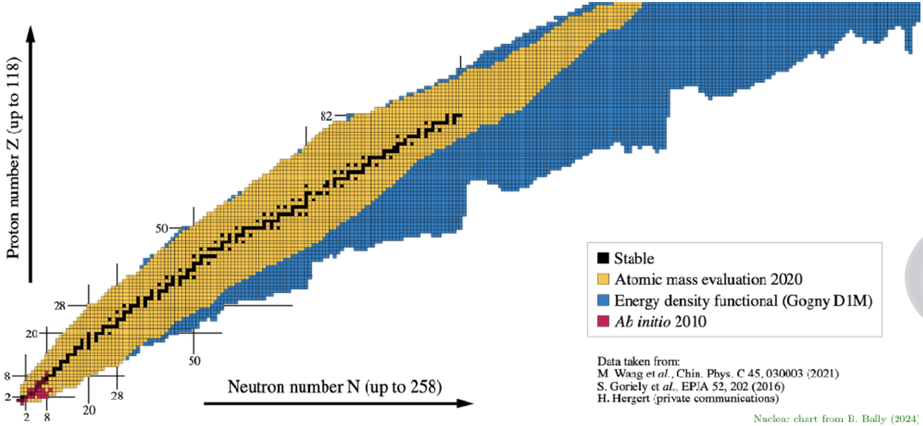
# Larger coverage with mean-field theory (Density Functional Theory)



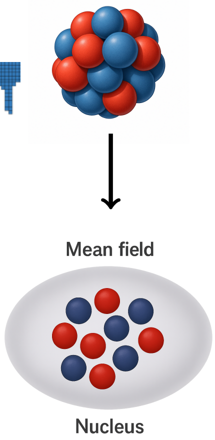



# Larger coverage with mean-field theory (Density Functional Theory)

Still structure only!



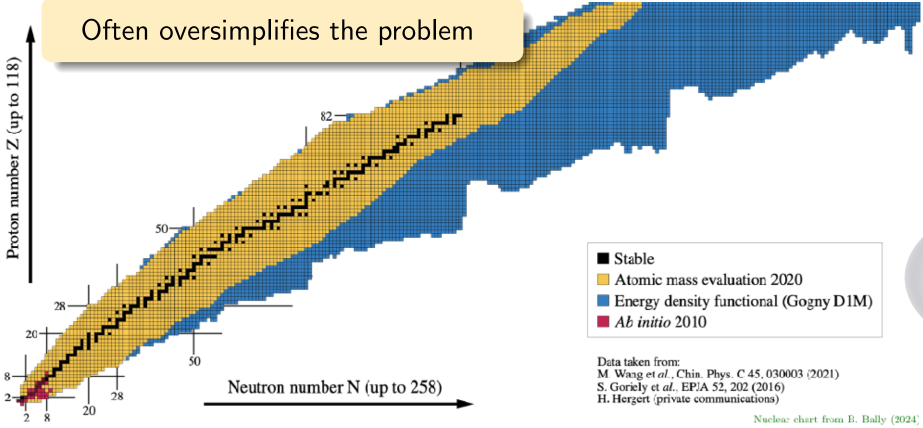

Nuclear chart from B. Bally (2024)

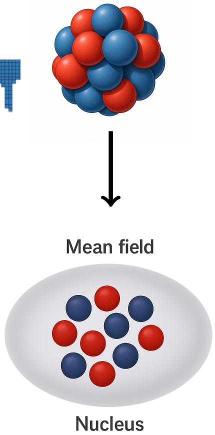


# Larger coverage with mean-field theory (Density Functional Theory)

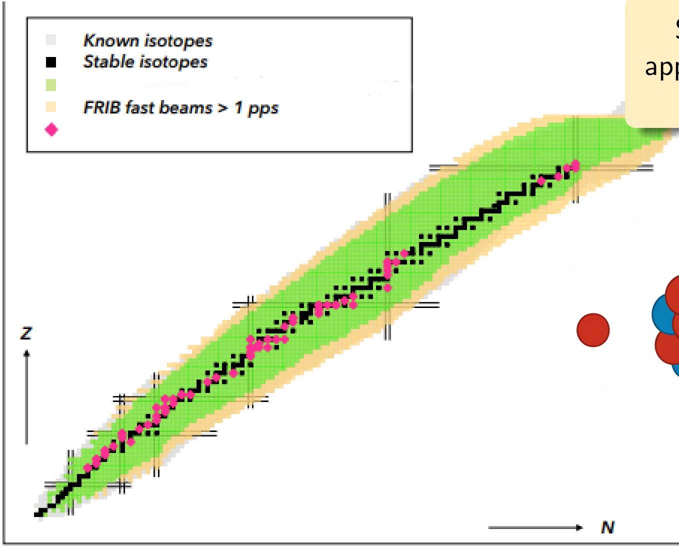
Still structure only!

Often oversimplifies the problem

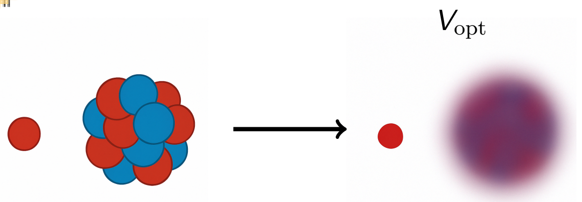


# Scattering and structure are typically treated separately → not ideal!




Standard Optical Potentials are applied across the nuclear chart, but lack nuclear structure




C. Hebborn *et al.*, J. of Phys. G **50**, 060501 (2023)

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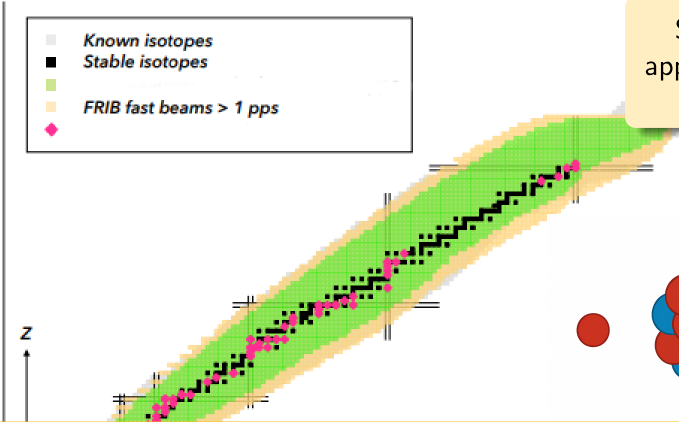


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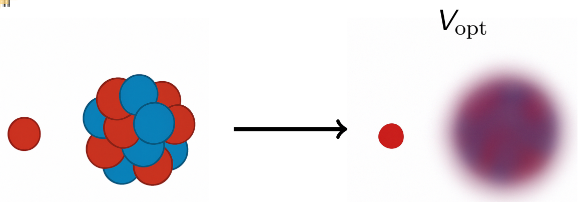


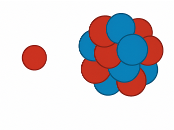

## Dispersive Optical Model

*The DOM strikes a balance between computational cost and a consistent treatment of bound and continuum dynamics*

C. Hebborn *et al.*, J. of Phys. G **50**, 060501 (2023)

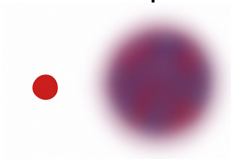
# Dispersive Optical Model (DOM): uniting structure and continuum

**Exact**

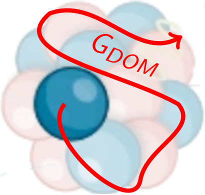


**DOM**

$\mathbf{V_{opt}}$

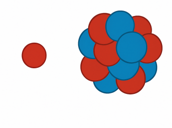


# Dispersive Optical Model (DOM): uniting structure and continuum




$G_{\mathrm{DOM}}$: Single-Particle Propagator

**Exact**



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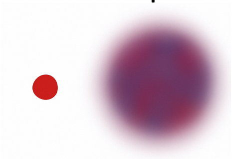

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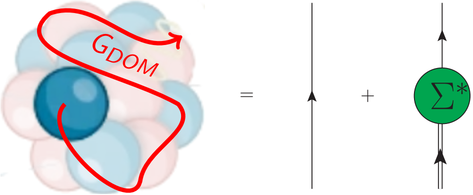
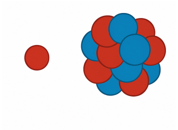


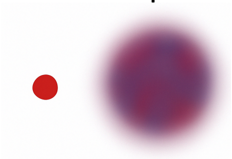

$G_{\text{DOM}}$: Single-Particle Propagator

**Exact**



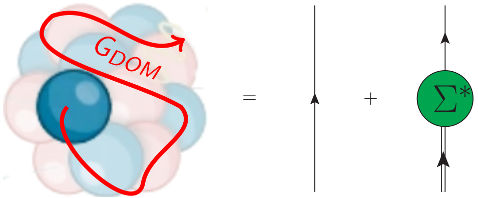
**DOM**

**$V_{\text{opt}}$**



# Dispersive Optical Model (DOM): uniting structure and continuum

- Self-energy: $\Sigma^*(r, r'; E) = V_{\text{opt}}(r, r'; E)$

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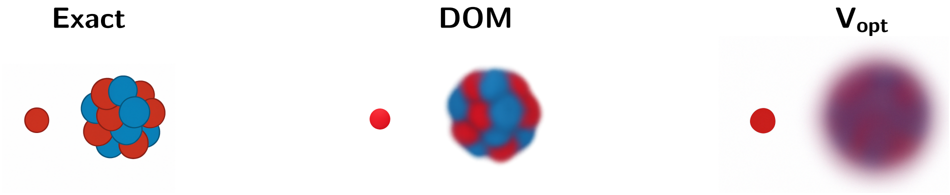
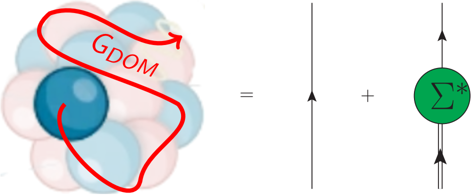


# Dispersive Optical Model (DOM): uniting structure and continuum

- Self-energy: $\Sigma^*(r, r'; E) = V_{\text{opt}}(r, r'; E)$

## Dispersive Correction

$$Re\Sigma_{\ell j}(r, r'; E) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} dE' \frac{Im\Sigma_{\ell j}(r, r'; E')}{E - E'}$$

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**Exact** **DOM** **$V_{opt}$**

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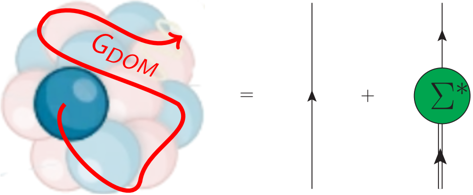
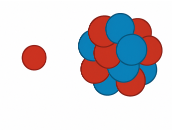



$G_{\rm DOM}$: Single-Particle Propagator

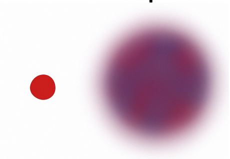
- This constraint ensures bound and scattering quantities are simultaneously described

**Exact**



**DOM**

**$\mathbf{V_{opt}}$**



# Constraining the self-energy of $^{40}$Ca

- Parameters of self-energy varied to minimize $\chi^2$

M.C. Atkinson *et al.*, PRC **98**, 044627 (2018)

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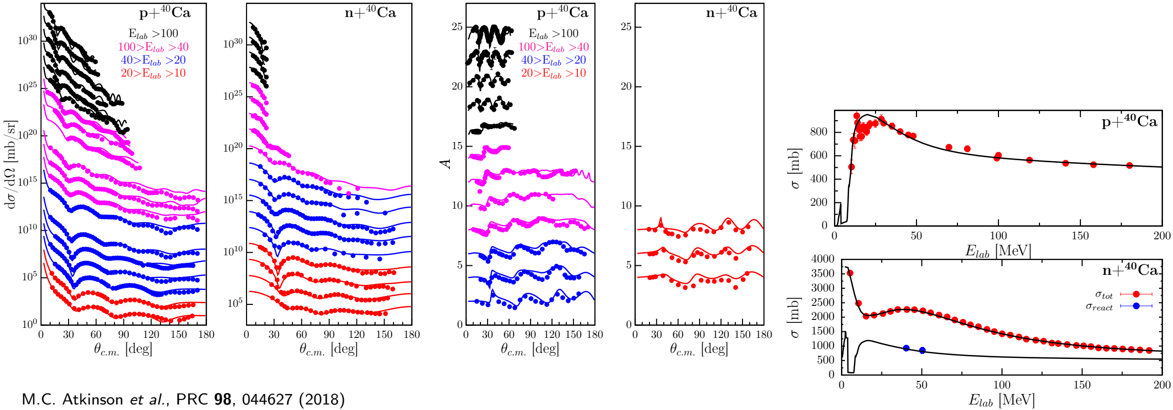


M.C. Atkinson *et al.*, PRC **98**, 044627 (2018)

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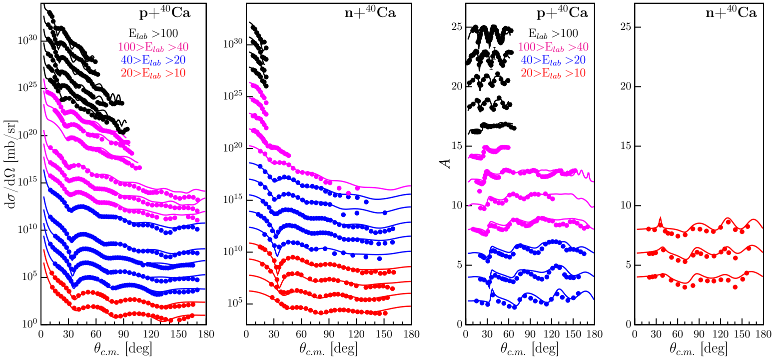
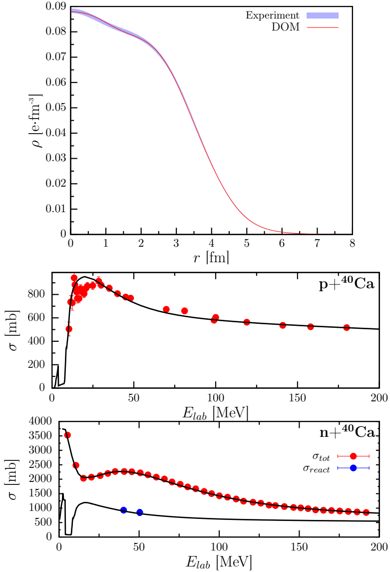
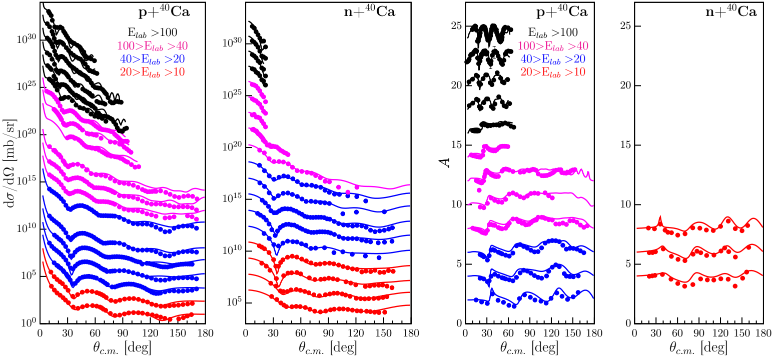


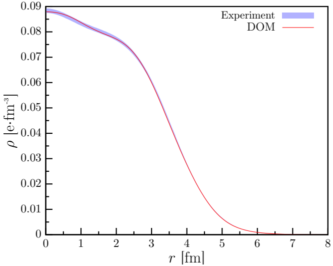



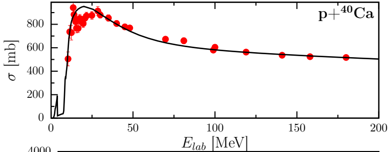

M.C. Atkinson *et al.*, PRC **98**, 044627 (2018)

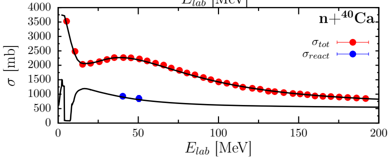
# Constraining the self-energy of $^{40}$Ca

- Parameters of self-energy varied to minimize $\chi^2$
- Reproducing the data ensures an accurate self-energy



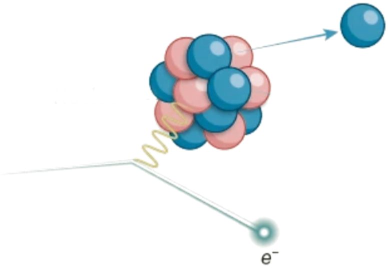




M.C. Atkinson *et al.*, PRC **98**, 044627 (2018)

# Electron scattering: the exclusive $^{40}Ca(e, e'p)^{39}K$ reaction

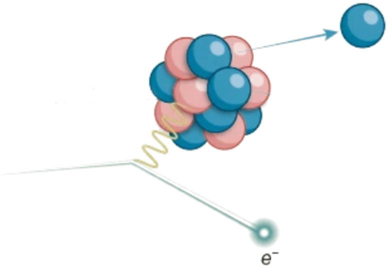
- Electron interaction means clean knockout reactions




M.C. Atkinson *et al.*, PRC **98**, 044627 (2018)

# Electron scattering: the exclusive $^{40}\mathrm{Ca}(e, e'p)^{39}\mathrm{K}$ reaction

- Electron interaction means clean knockout reactions
- Cross section is closely tied to the boundstate wavefunction




M.C. Atkinson *et al.*, PRC **98**, 044627 (2018)

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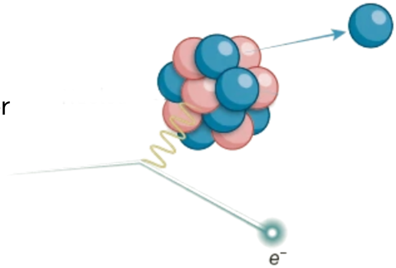
- Evidence of physics beyond mean-field: Spectroscopic Factor




M.C. Atkinson *et al.*, PRC **98**, 044627 (2018)

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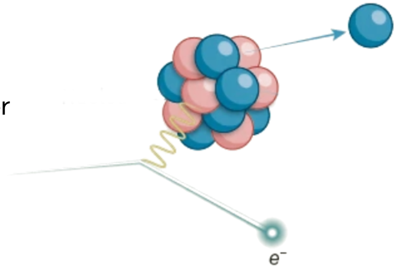
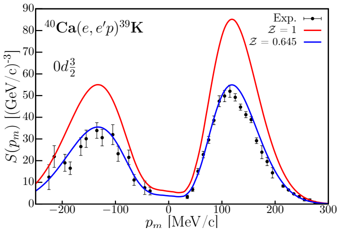


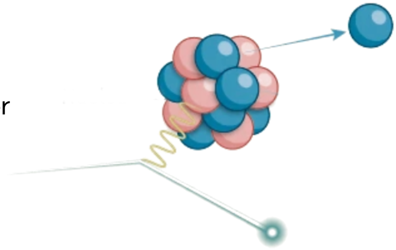

**Old Mean-Field**



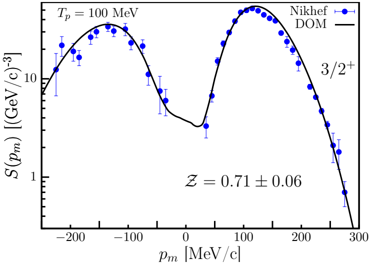

M.C. Atkinson *et al.*, PRC **98**, 044627 (2018)

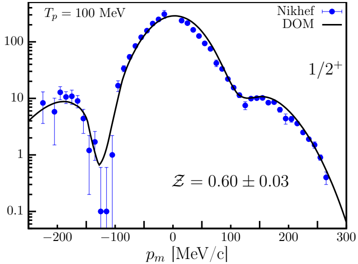
# Electron scattering: the exclusive $^{40}$Ca$(e, e'p)^{39}$K reaction

- Electron interaction means clean knockout reactions
- Cross section is closely tied to the boundstate wavefunction
- Evidence of physics beyond mean-field: Spectroscopic Factor
- DOM allows first consistent calculation

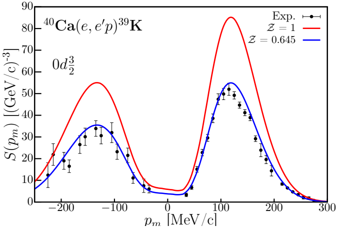



## DOM Prediction




## Old Mean-Field




M.C. Atkinson *et al.*, PRC **98**, 044627 (2018)

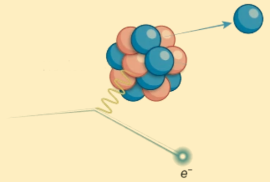
# Now consider knockout with a hadronic probe: $^{40}\mathrm{Ca}(p,2p)^{39}\mathrm{K}$

- Proton knockout can be used in both stable and exotic nuclei

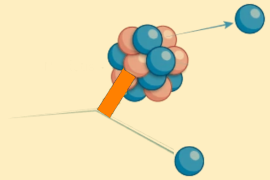
M.C. Atkinson *et al.*, Front. Phys. **12**, 1505982 (2025)

M.C. Atkinson *et al.*, PRC **105**, 014622 (2022)

## Electron probe: $^{40}\mathrm{Ca}(e,e'p)^{39}\mathrm{K}$




## Proton probe: $^{40}\mathrm{Ca}(p,2p)^{39}\mathrm{K}$



# Now consider knockout with a hadronic probe: $^{40}\mathrm{Ca}(p,2p)^{39}\mathrm{K}$

- Proton knockout can be used in both stable and exotic nuclei

M.C. Atkinson *et al.*, Front. Phys. **12**, 1505982 (2025)

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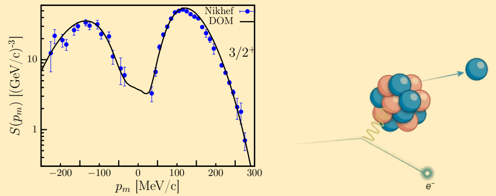


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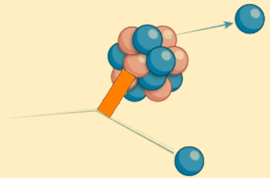

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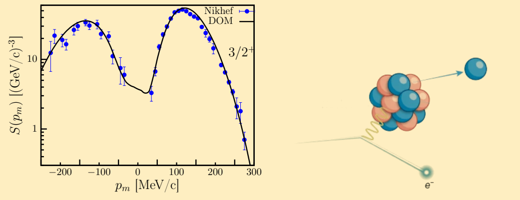


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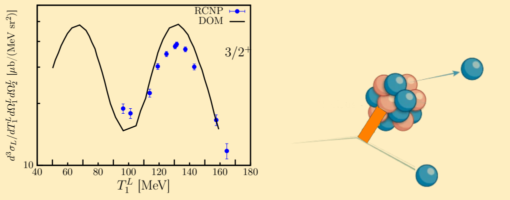
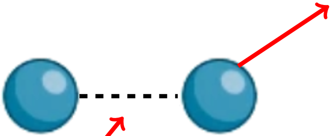


# Now consider knockout with a hadronic probe: $^{40}\text{Ca}(p,2p)^{39}\text{K}$

- Proton knockout can be used in both stable and exotic nuclei
- Discrepancy caused by using free $V_{pp}$



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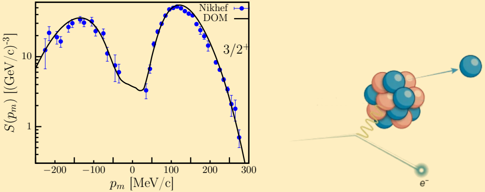


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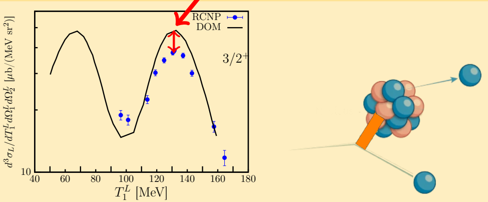
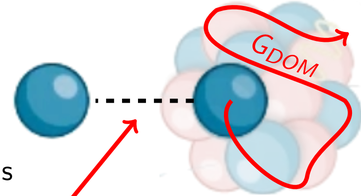


# Now consider knockout with a hadronic probe: $^{40}\mathrm{Ca}(p,2p)^{39}\mathrm{K}$

- Proton knockout can be used in both stable and exotic nuclei
- Discrepancy caused by using free $V_{pp}$
- Dress $V_{pp}$ to include effect of proton propagating through nucleus (propagator $G_{DOM}$)

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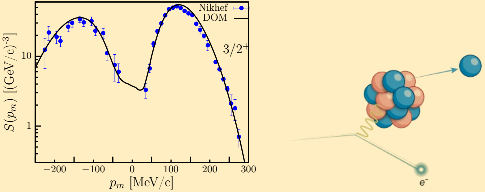


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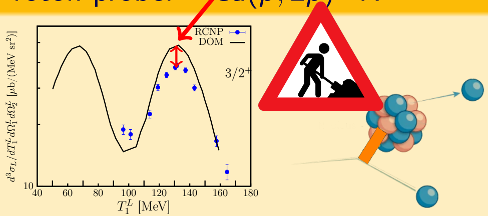
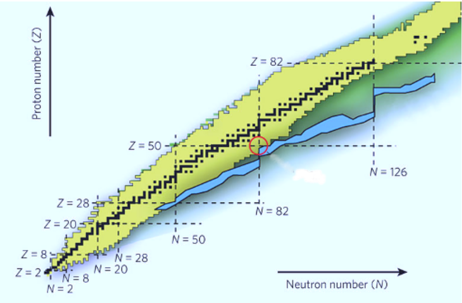
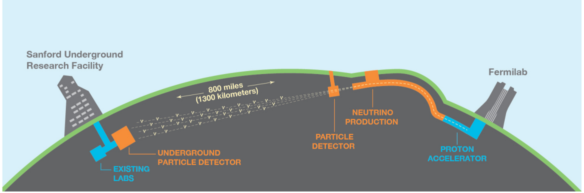
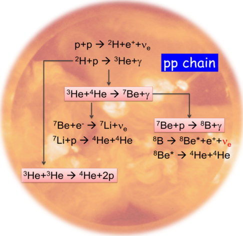


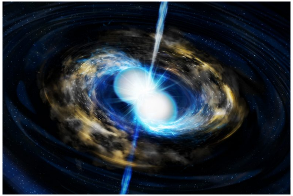
# Outlook

- Use dressed $V_{pp}$ in reactions throughout nuclear chart
- Synergizes with global DOM effort
  - Reactions with exotic nuclei (e.g. $^{52}$Ca)
- Investigate $e$ and $\nu$ scattering with $^{40}$Ar for DUNE
- Work already begun to analyze JLab experiment on $^{40}\mathrm{Ar}(e, e'p)^{39}\mathrm{Cl}$
- Investigate impact of $V_{NN}$ on Helium fusion



# Thanks

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