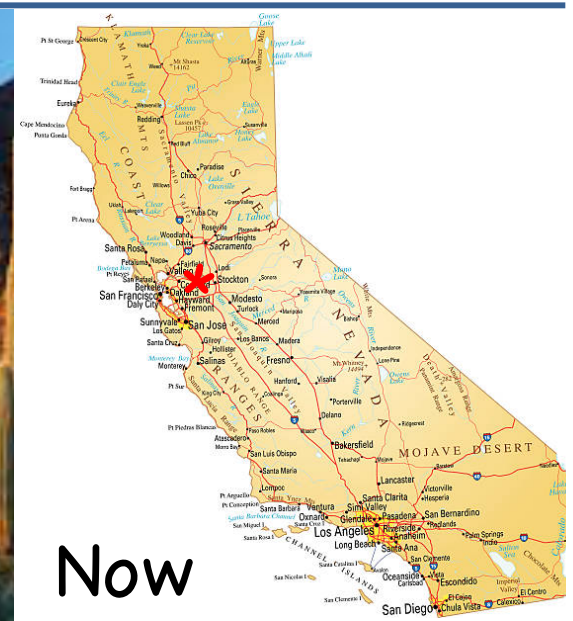


# Light and unbound nuclei

Rewriting Nuclear Physics Textbooks: Basic nuclear interactions and their link to nuclear processes in the cosmos and on earth

Pisa, July 25, 2017

Sofia Quaglioni



# Content

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- What are light and unbound nuclei?
- What is the role of light and unbound nuclei in the Cosmos and on Earth?
- How can we learn about the basic nuclear interactions?
- Can we describe exotic nuclei and the phenomena of low-energy nuclear reactions?

What are light and  
unbound nuclei?





# Binding energy (BE)

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- The energy required to disintegrate a nucleus into its components

$$BE(Z, N) = Z m_p c^2 + N m_n c^2 - M(Z, N) c^2$$

- Progressively adding neutrons (protons) drives the binding energy to zero: driplines

# The case of ${}^5\text{He}$

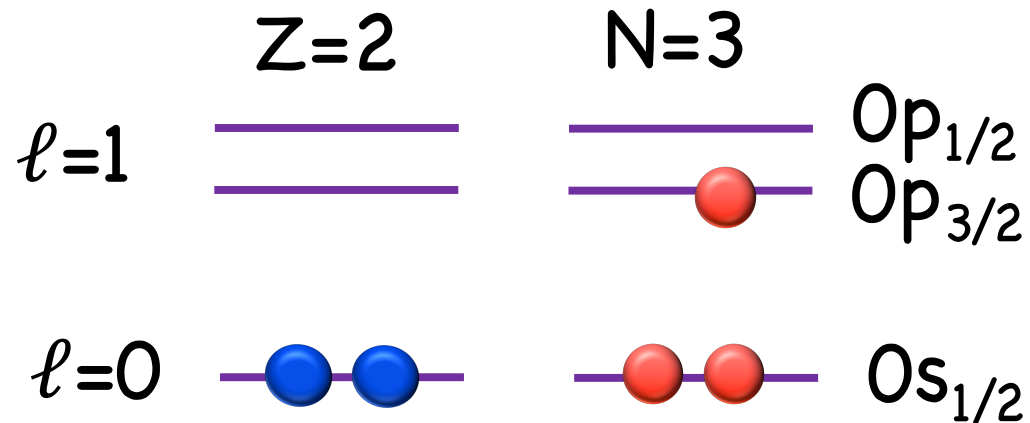
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- ${}^4\text{He}$  tightly bound (BE = 28.30 MeV)
- ${}^5\text{He}$  is not bound. Why?!?

# The case of ${}^5\text{He}$

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## 1) Pauli exclusion principle

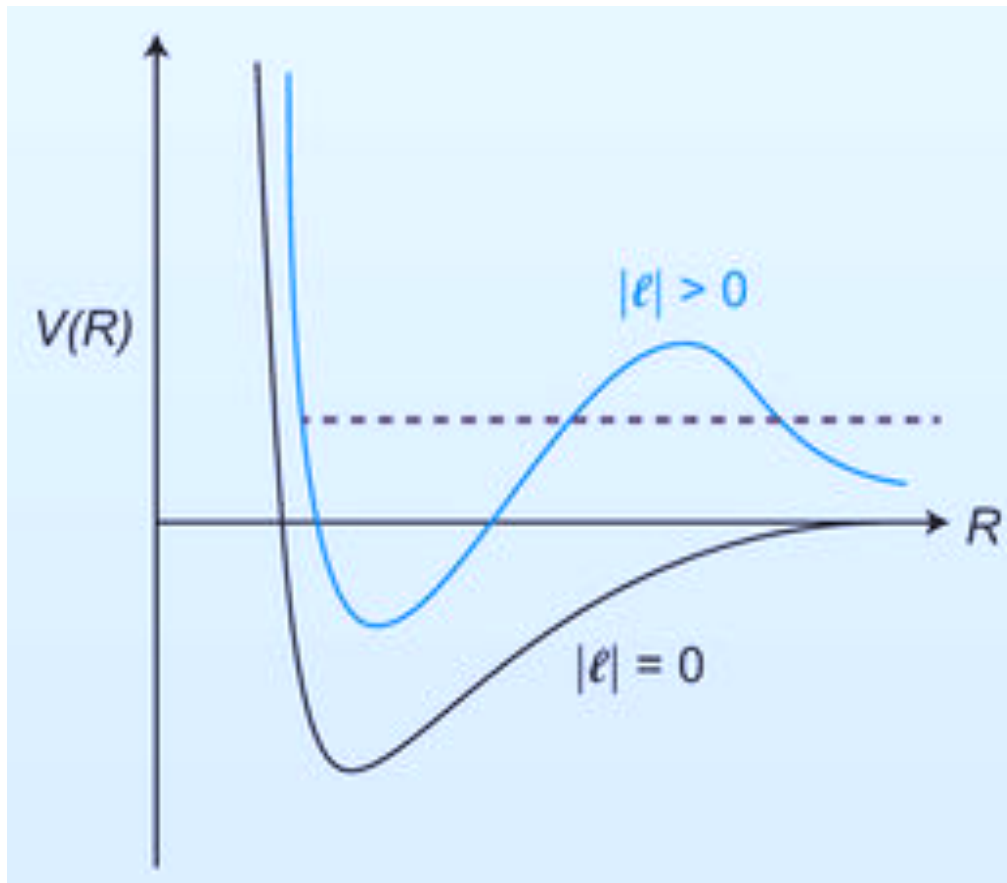


s-shell is full, extra neutron must be in p shell



# The case of ${}^5\text{He}$

## 2) Centrifugal barrier




Overall potential is attractive but not enough to bind the system

# Unbound nuclear systems, resonances


---

$$\psi(t, \mathbf{r}) = \exp\left(-\frac{iE}{\hbar}t\right)\psi(0, \mathbf{r})$$

Solution of  
time-dependent  
Schrodinger  
equation



Solution of  
time-**i**ndependent  
Schrodinger  
equation



# Unbound nuclear systems, resonances

---

$$\psi(t, \mathbf{r}) = \exp\left(-\frac{iE}{\hbar}t\right)\psi(0, \mathbf{r})$$

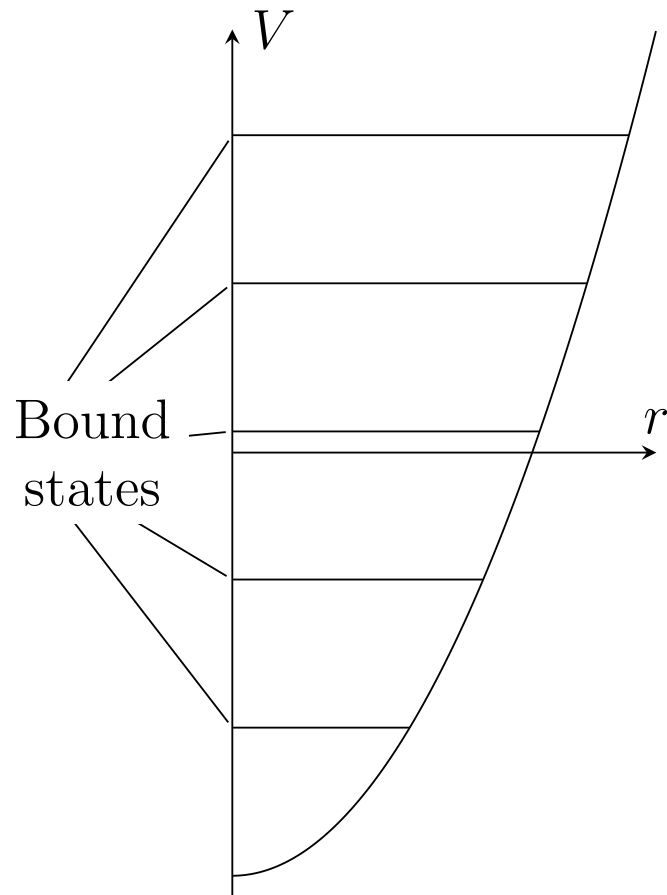
■ Energy  $E$  is a real number:  $|\psi(t, \mathbf{r})|^2 = |\psi(0, \mathbf{r})|^2$

■ Energy  $E$  is a complex complex:  $E = E_0 - i\frac{\Gamma}{2}$

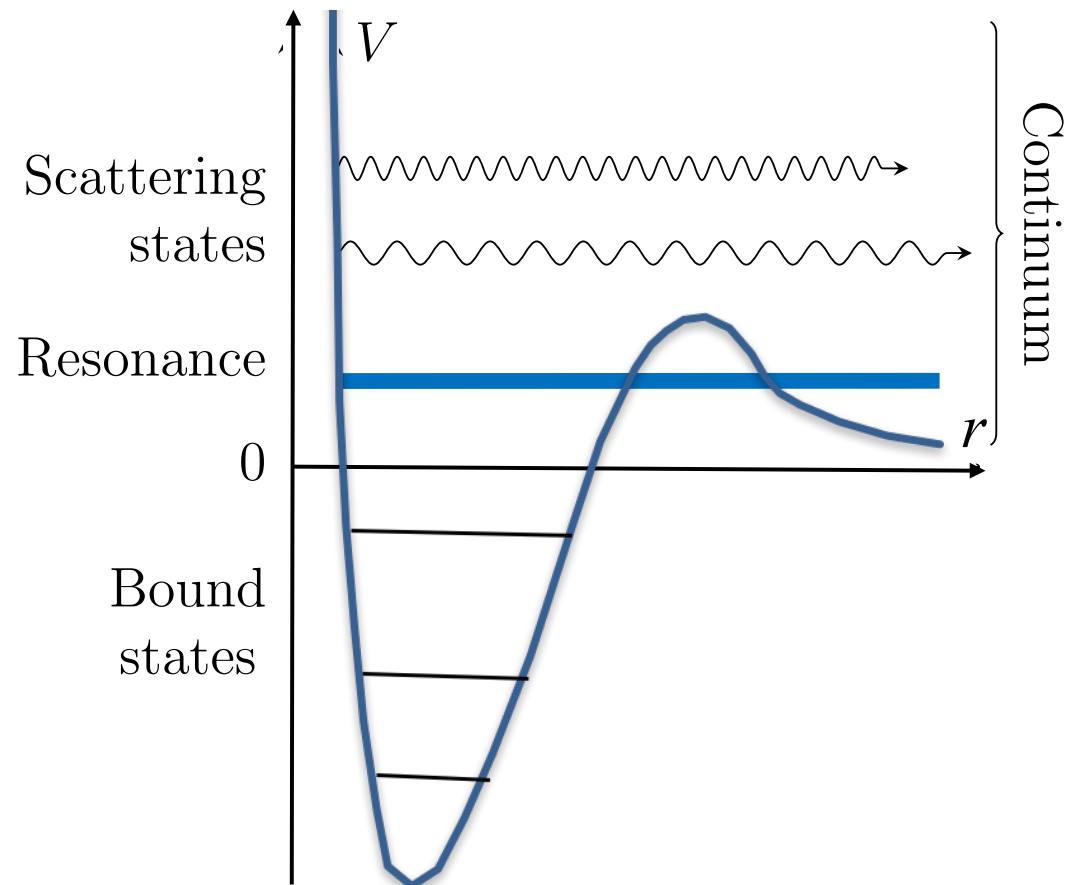
$$|\psi(t, \mathbf{r})|^2 = \exp\left(-\frac{\Gamma}{\hbar}t\right)|\psi(0, \mathbf{r})|^2$$

Resonance state  
decaying exponentially  
 $T_{1/2} = \ln 2 / \Gamma$

# Unbound nuclear systems, resonances



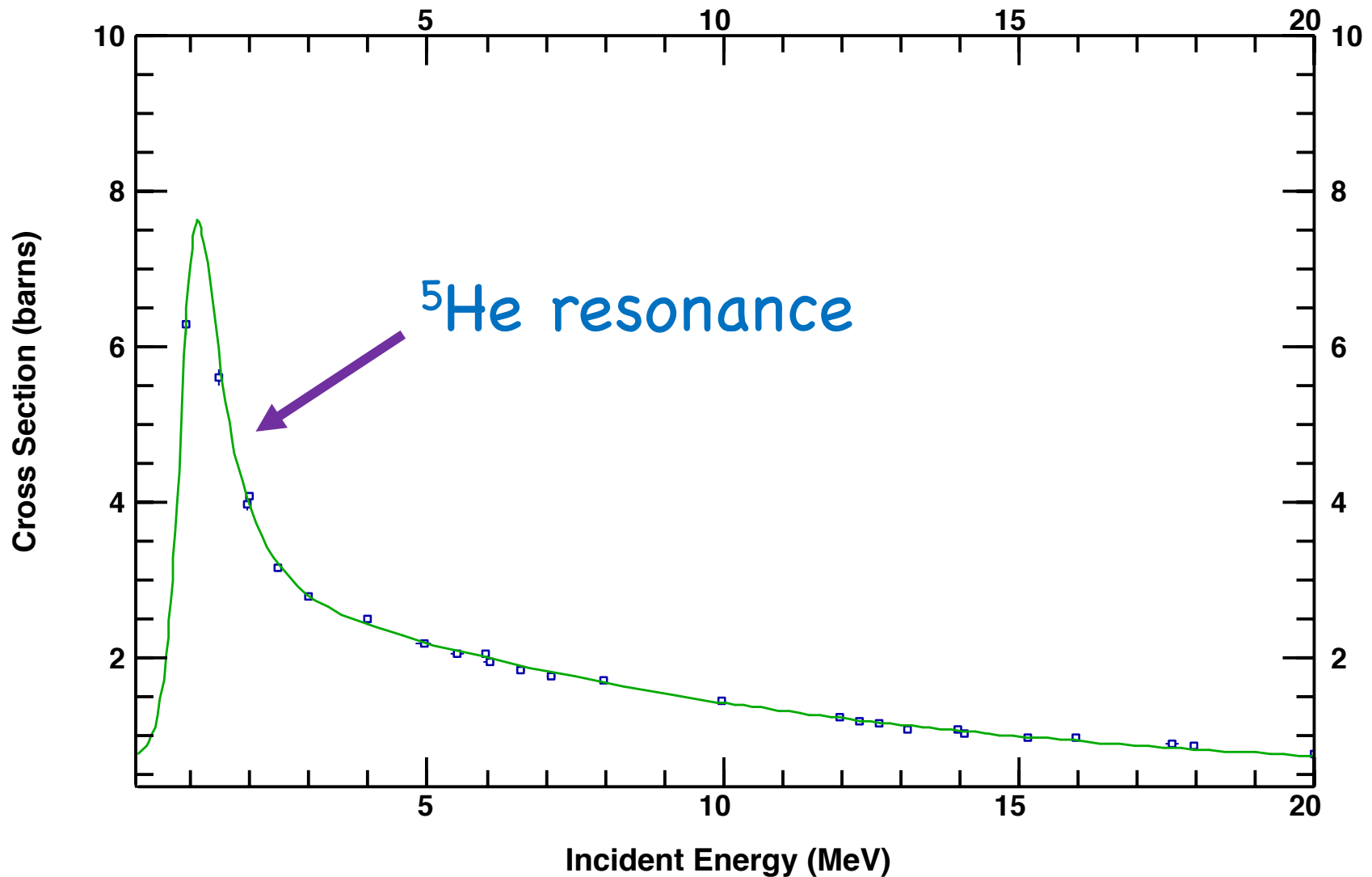
(a) A closed quantum system



(b) An open quantum system

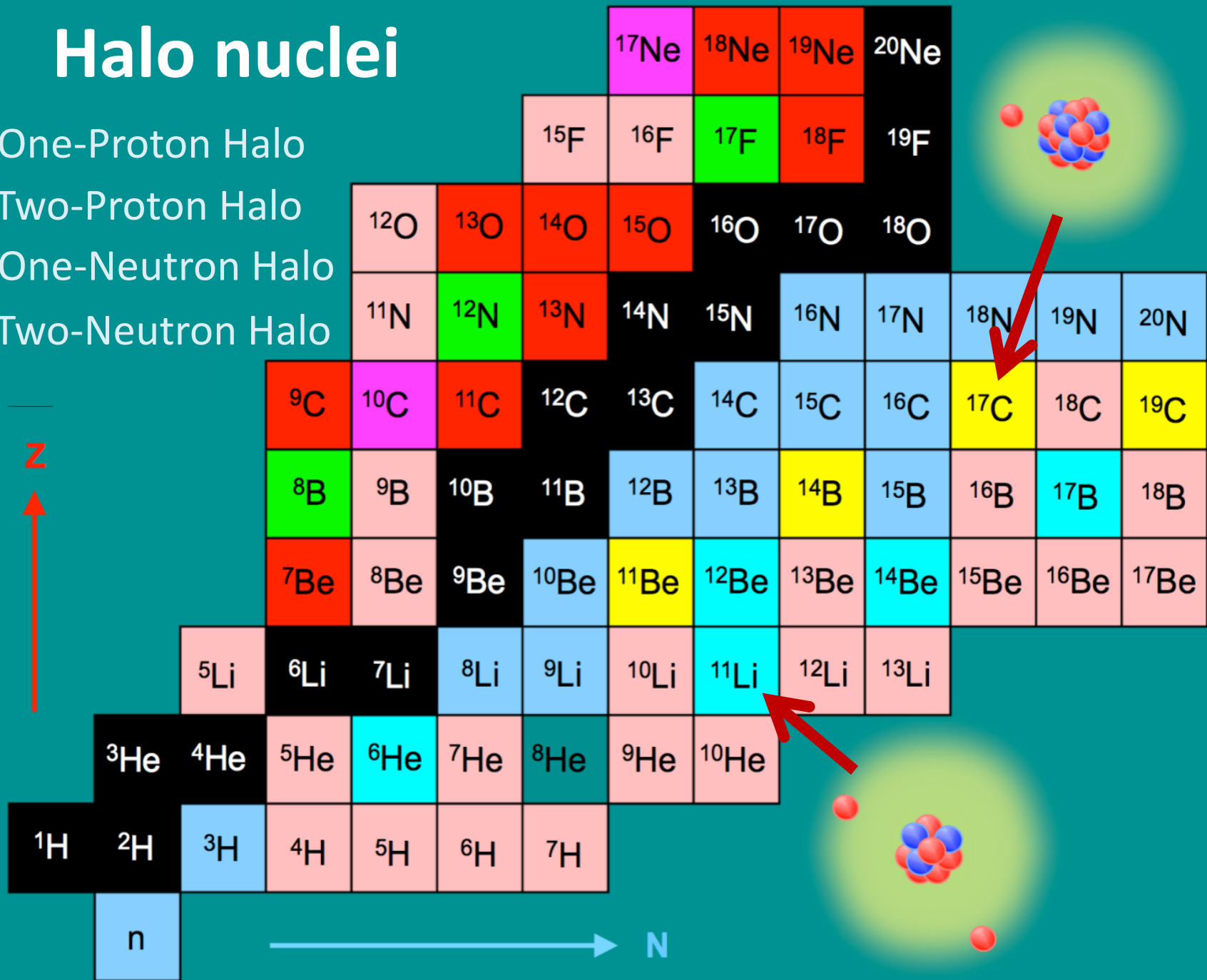
Adapted from J. Bengtsson, BS Thesis, Chalmers University

# Elastic scattering of neutrons on $^4\text{He}$

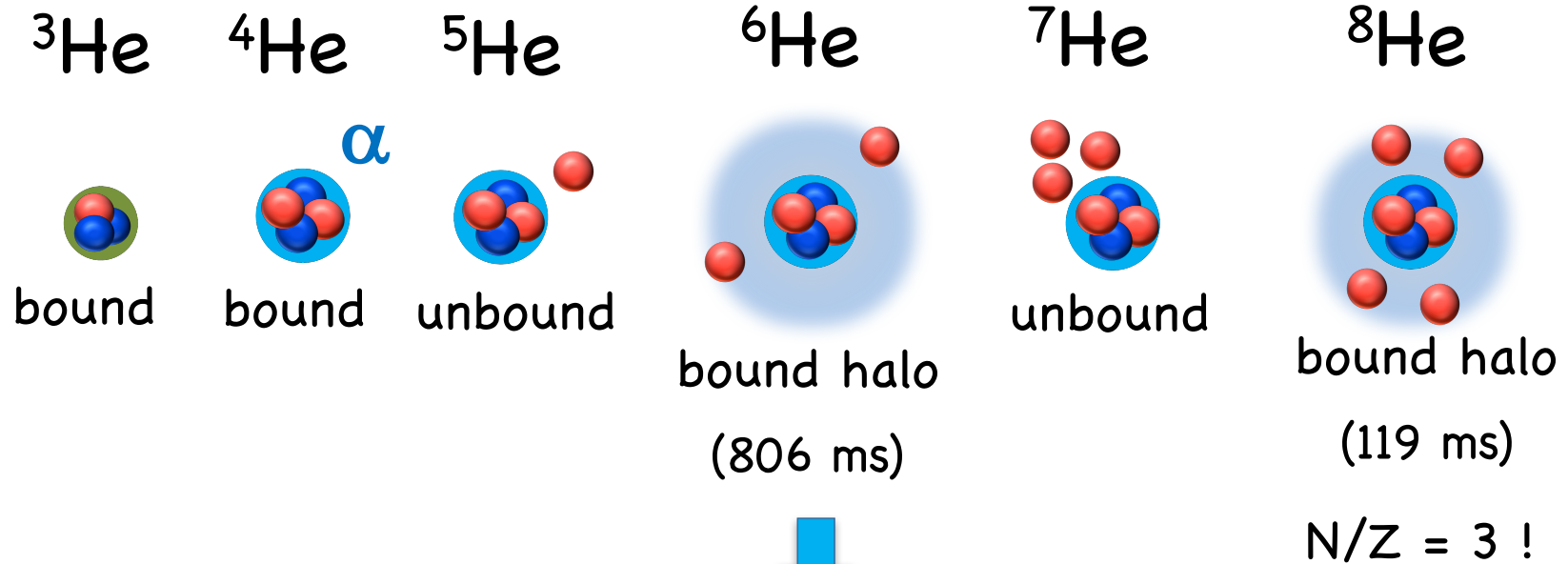


# Halo nuclei

- One-Proton Halo
- Two-Proton Halo
- One-Neutron Halo
- Two-Neutron Halo



# The helium isotopes chain



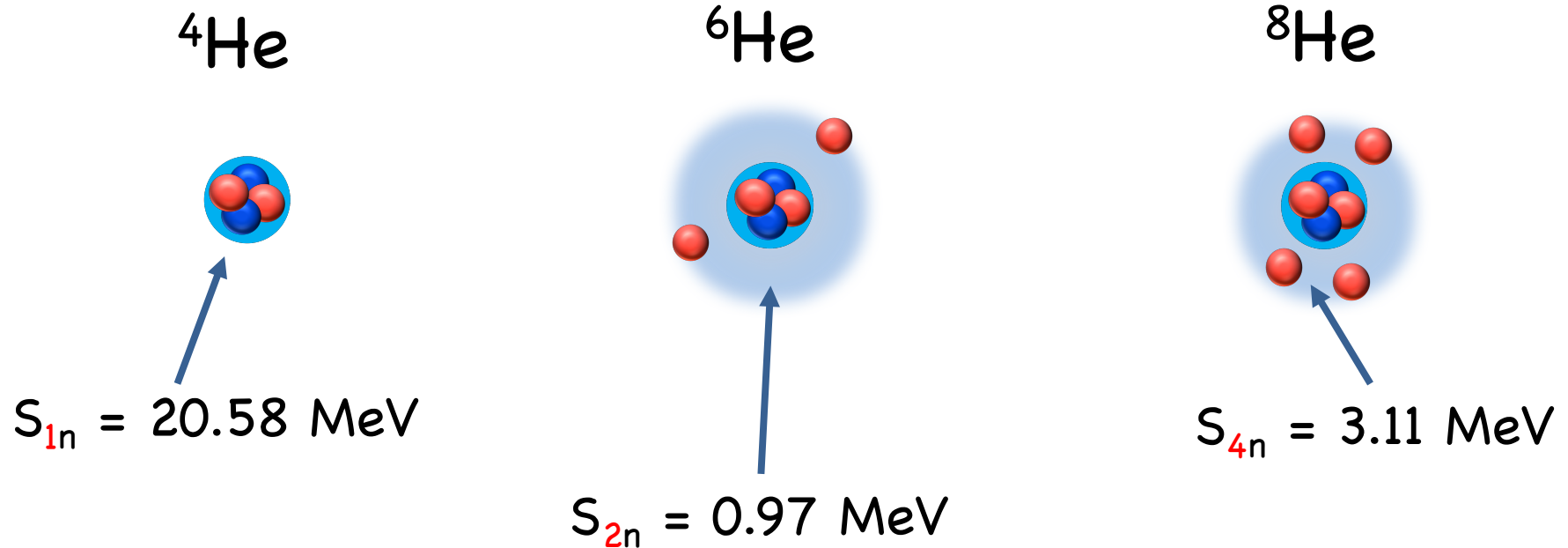
Borromean  
Halo



# Separation energy: energy required to separate particle(s)

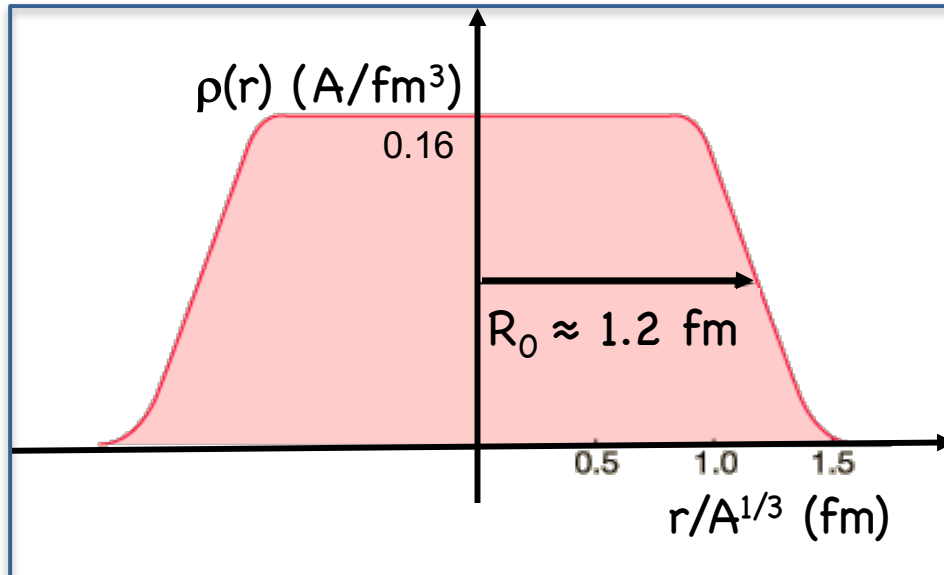
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$$S_{a_n}(Z,N) = BE(Z,N) - BE(Z,N-a)$$

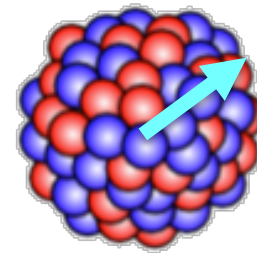




# Nuclear sizes



$^{208}\text{Pb}$

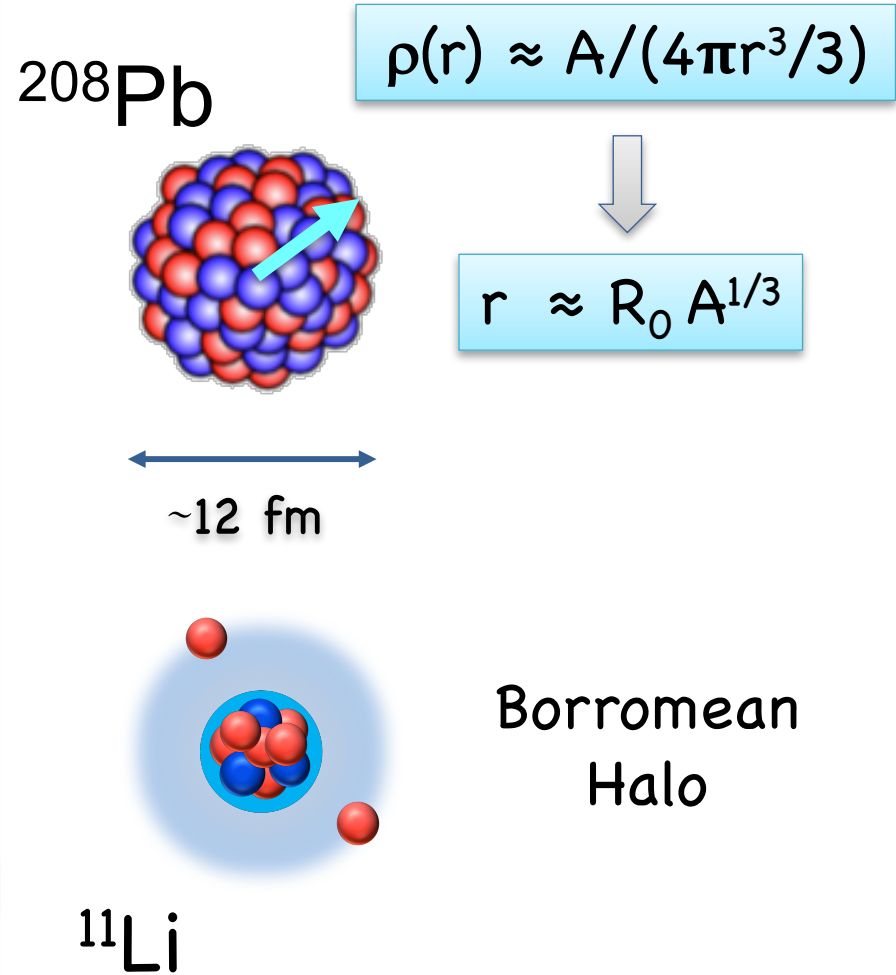
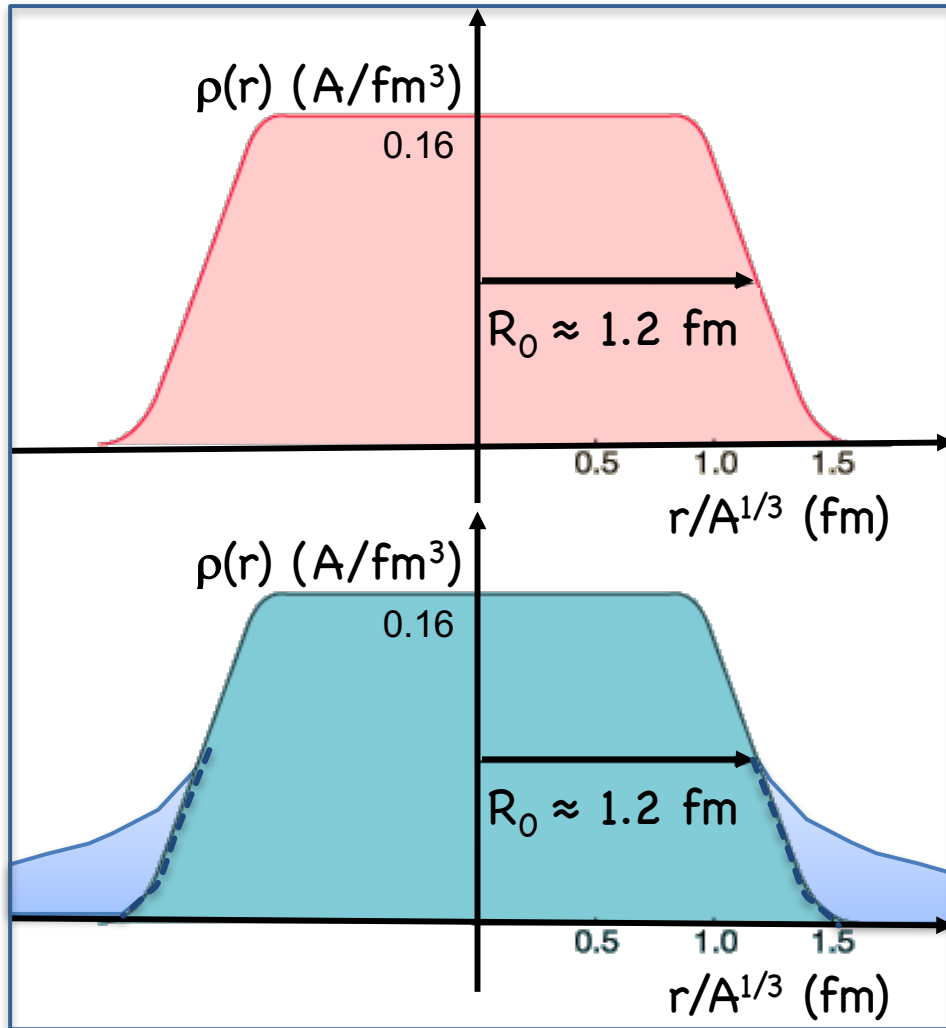


$$\rho(r) \approx A/(4\pi r^3/3)$$



$$r \approx R_0 A^{1/3}$$

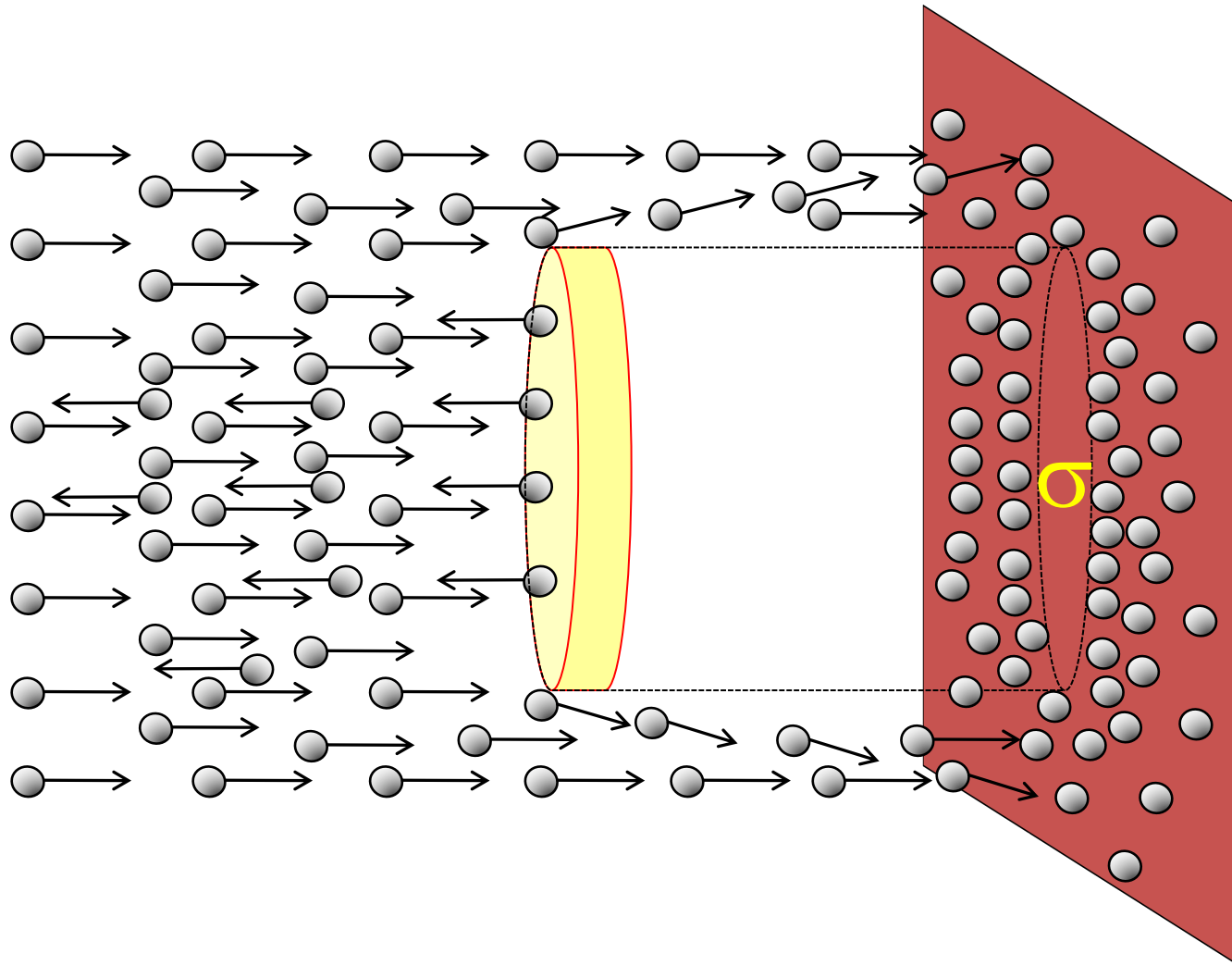
# Nuclear sizes



# How do we measure nuclear sizes?

## Cross section ( $\sigma$ ): a classical view

---



As big as a barn ...



$$1 \text{ barn} = 10^{-28} \text{ m}^2 = 100 \text{ fm}^2$$

# Summary

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- The vast majority of light nuclei are either unstable or not bound
- Nuclear physics does not stop at binding energies and radii
- **All** observed nuclear phenomena can help us understand the basic nuclear interactions
- Light nuclei already display a wide variety of phenomena

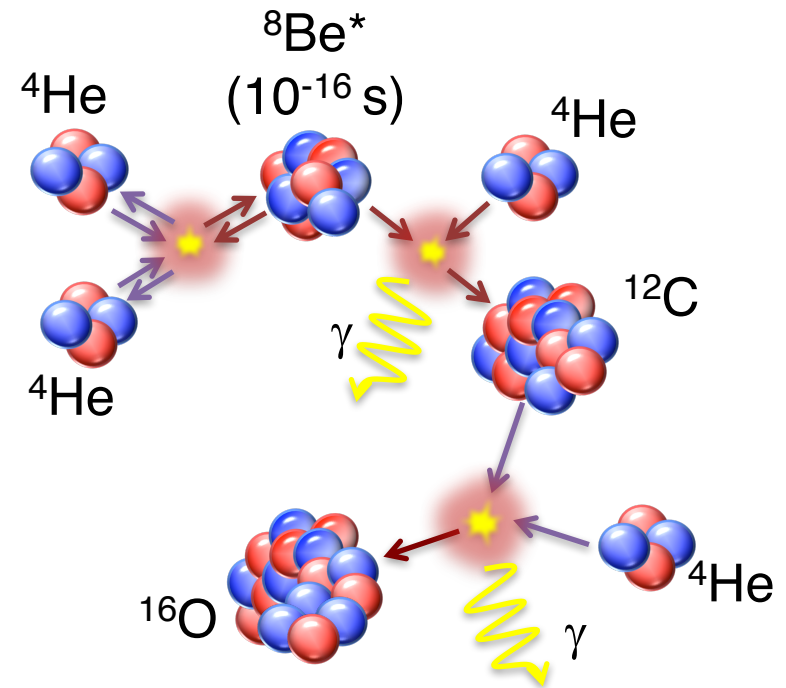
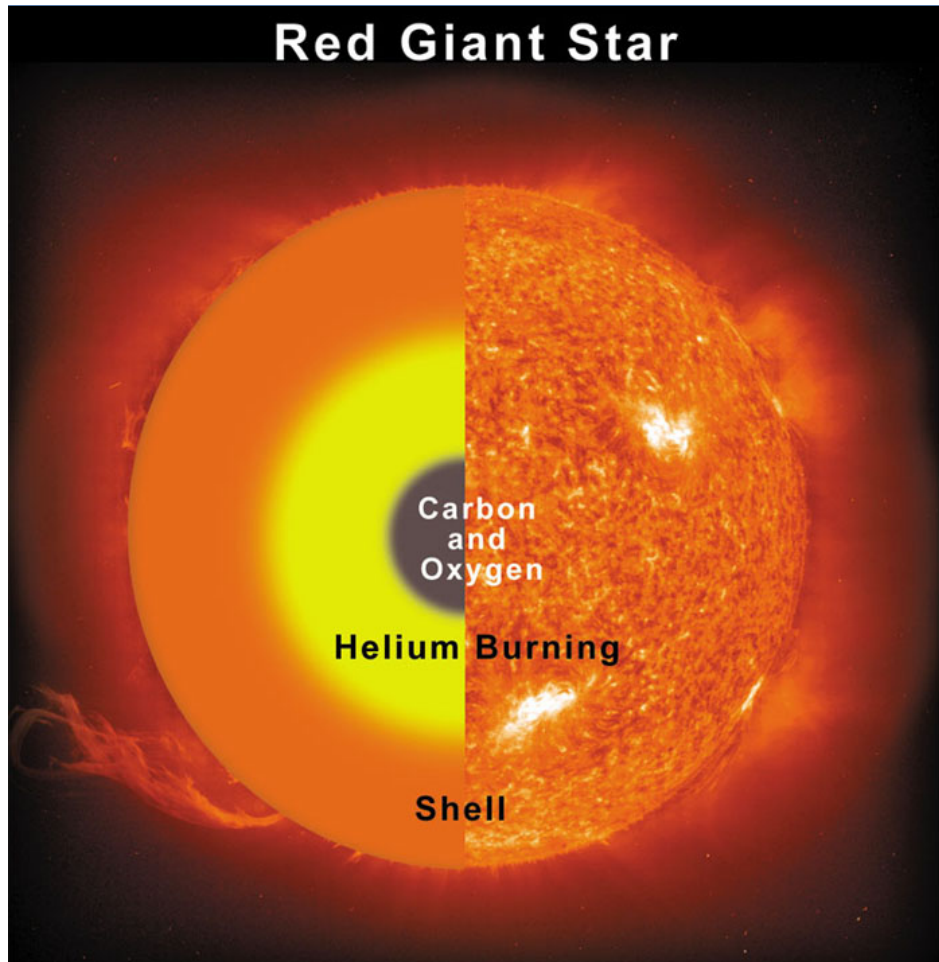
# Questions

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- Do you have any question so far?
- Form a group of 2 or 3 people and take a couple of minutes to discuss ...

What is the role of light  
and unbound nuclei in the  
Cosmos and on Earth?

# Reactions 'R' Us

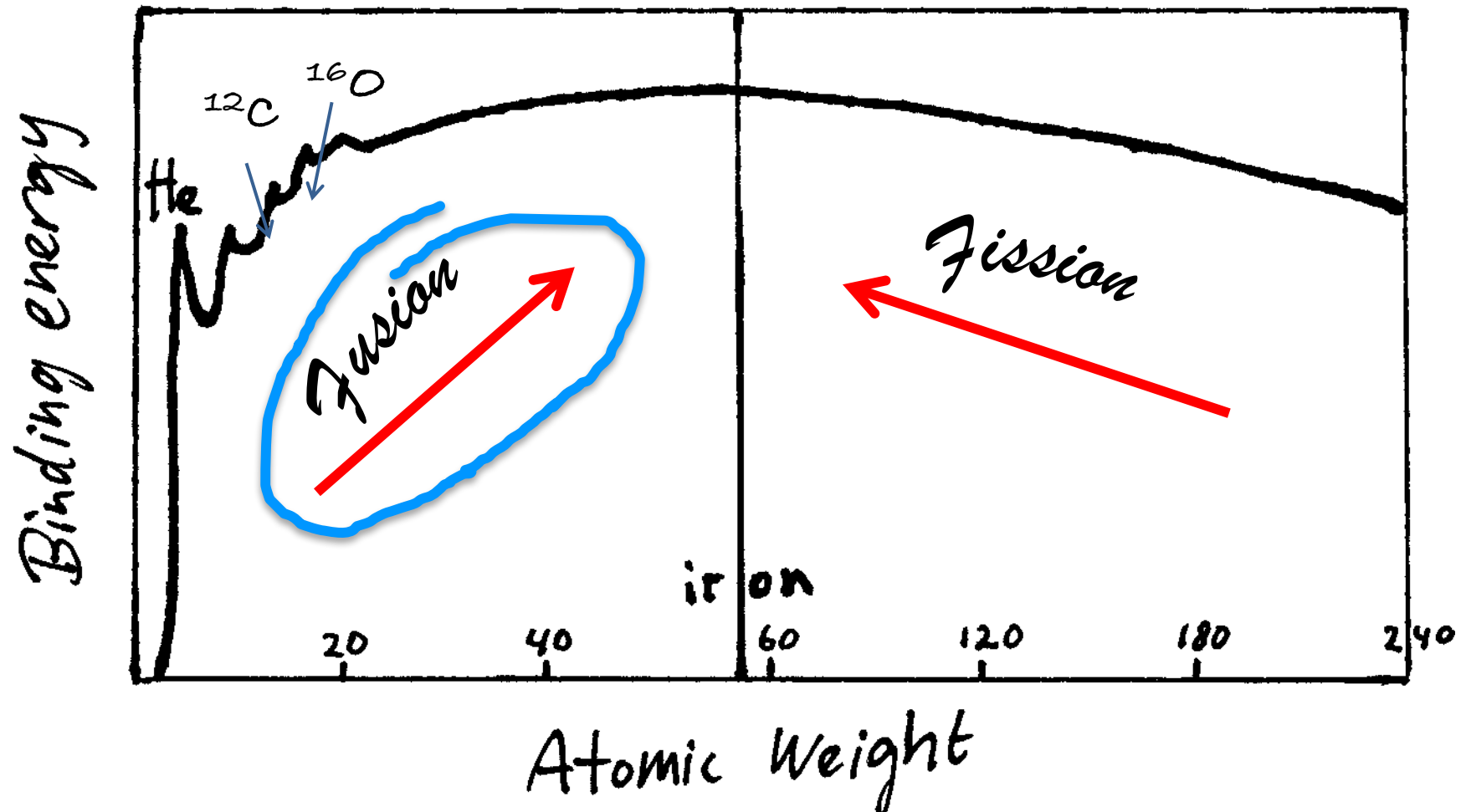


From light and unbound nuclei to the the chemical building blocks of life, to the processes that shaped our Universe



# Stars are powered by thermonuclear fusion reactions

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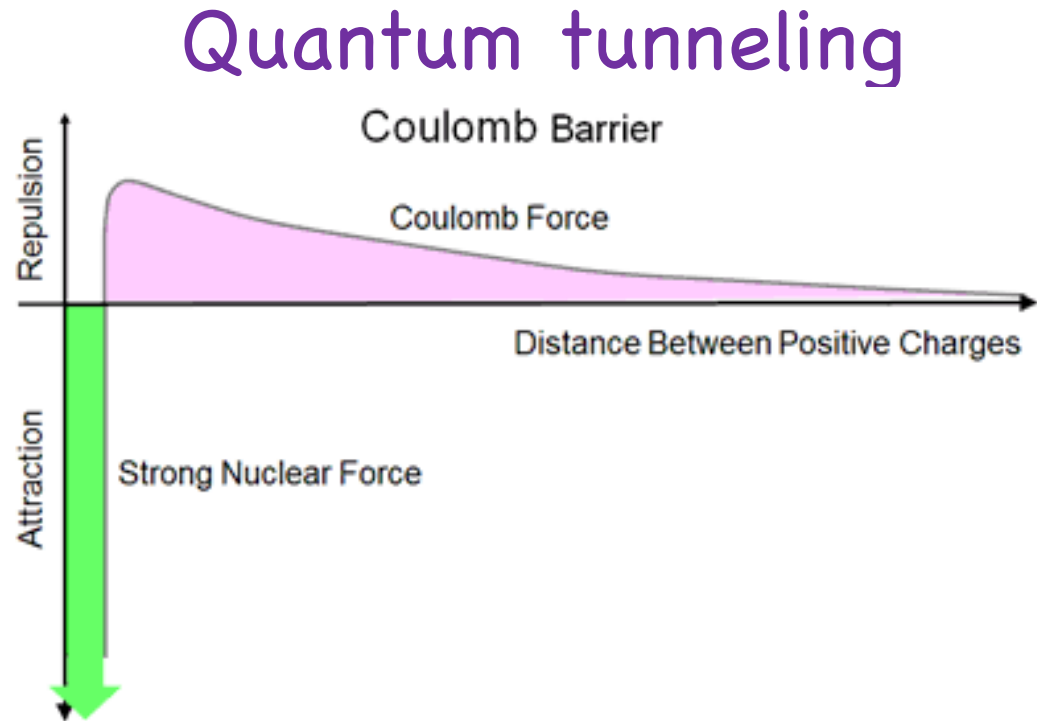


# Cross section of fusion reactions at stellar energies are very small !

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- Positively-charged colliding nuclei electrically repel each other

- Fusion process operates mainly by tunneling through the Coulomb barrier



# Fusion cross sections drop nearly exponentially with decreasing energy

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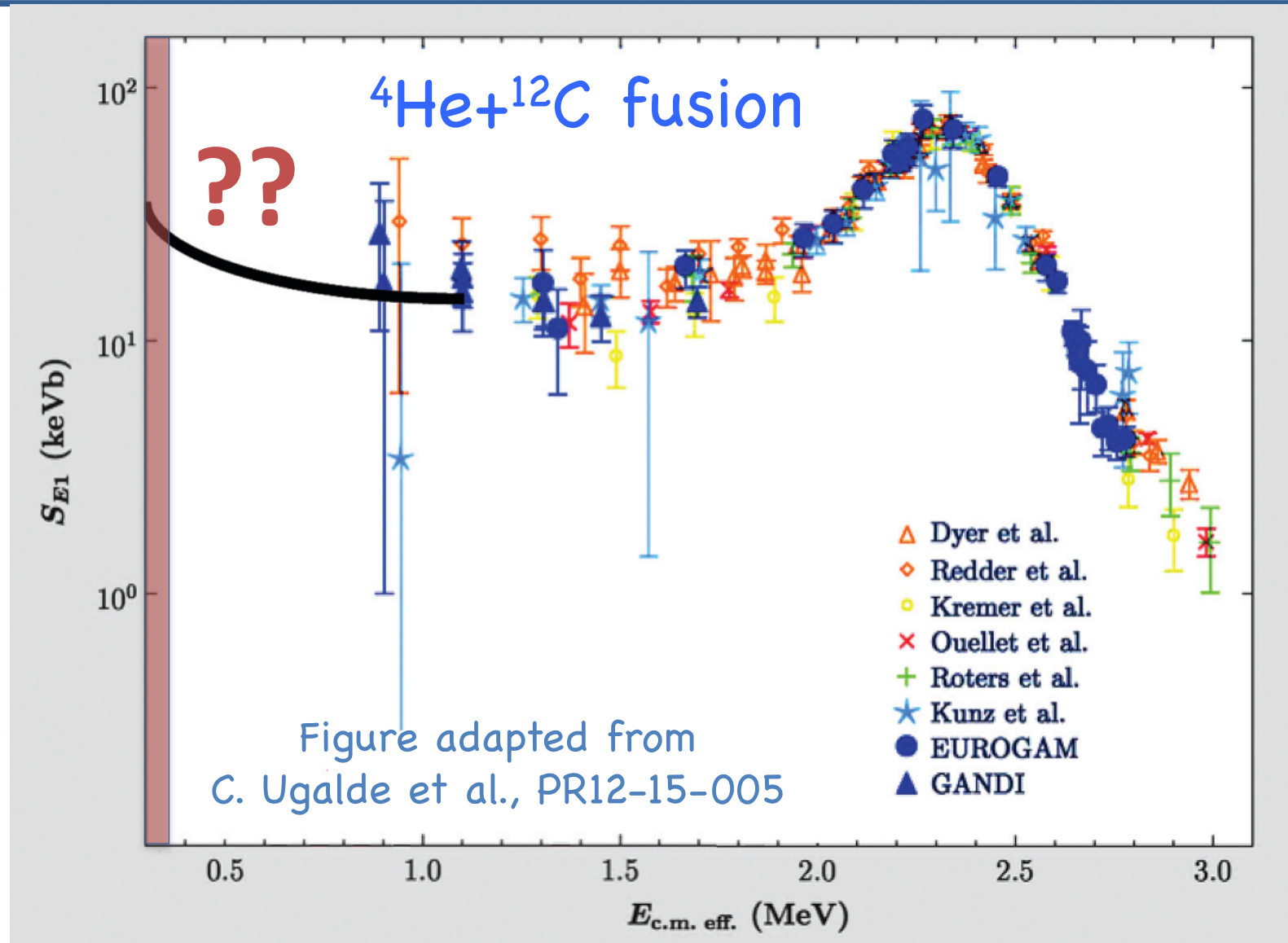
Fusion cross section

Astrophysical S-factor:  
nuclear contribution

$$\sigma(E) = \frac{S(E)}{E} \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2E/m}}\right)$$

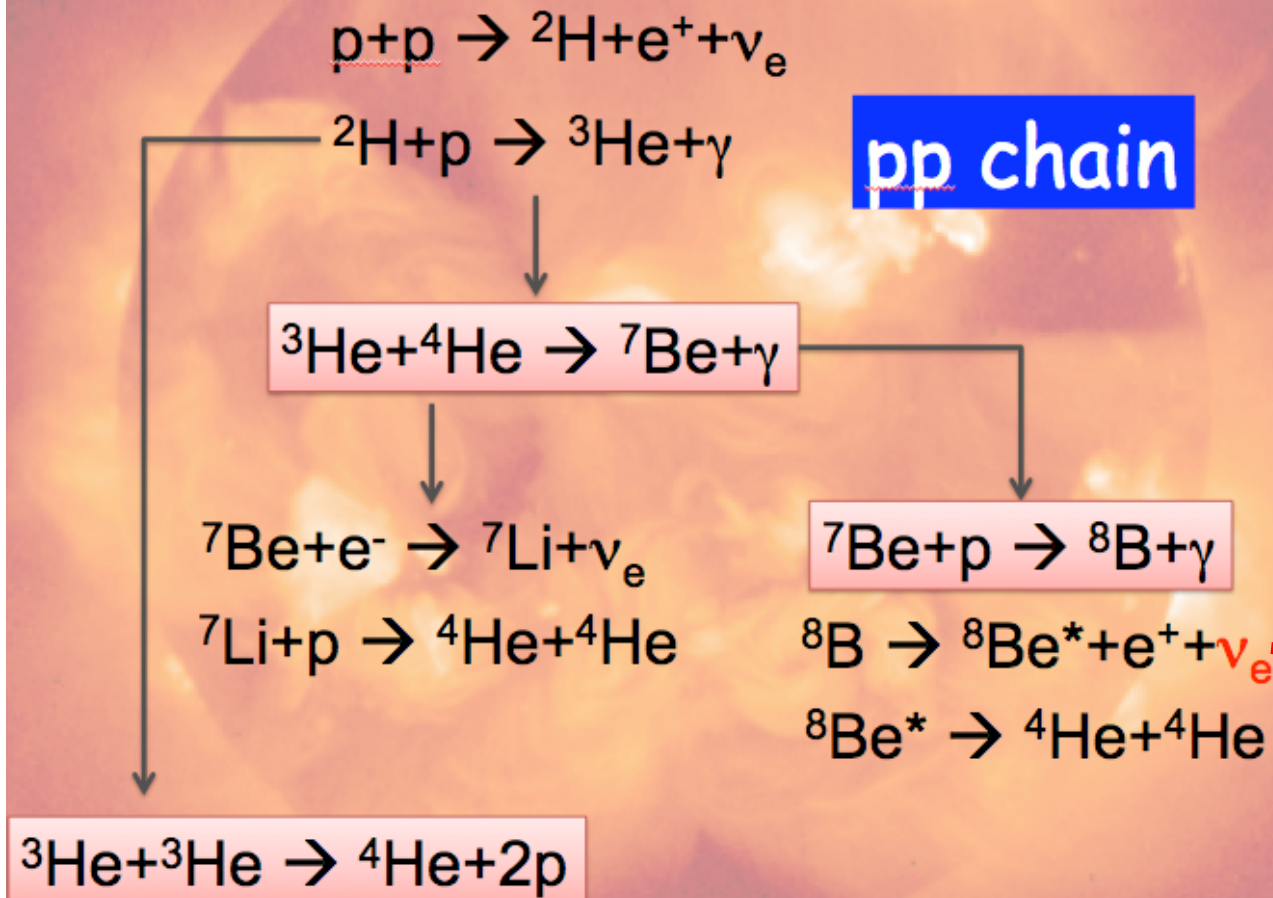
'Coulomb'  
Contribution  
(tunneling)

# We need reliable theory to estimate the S-factor at stellar energies

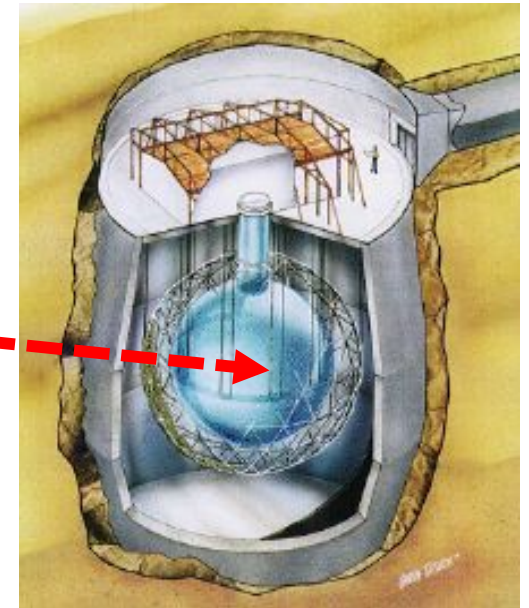


# Our Sun: one of the best tools for studying neutrinos

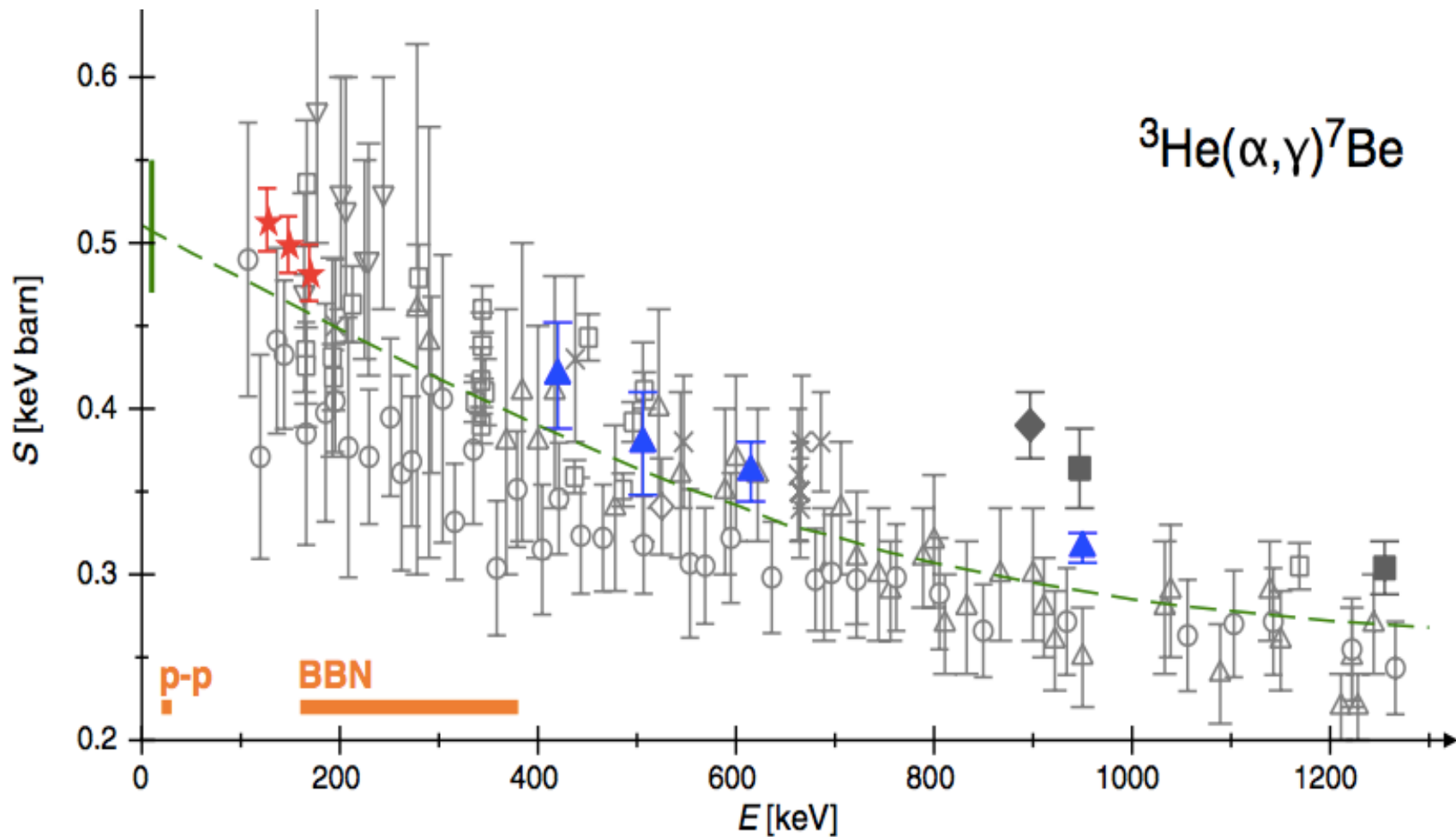
## Standard solar model



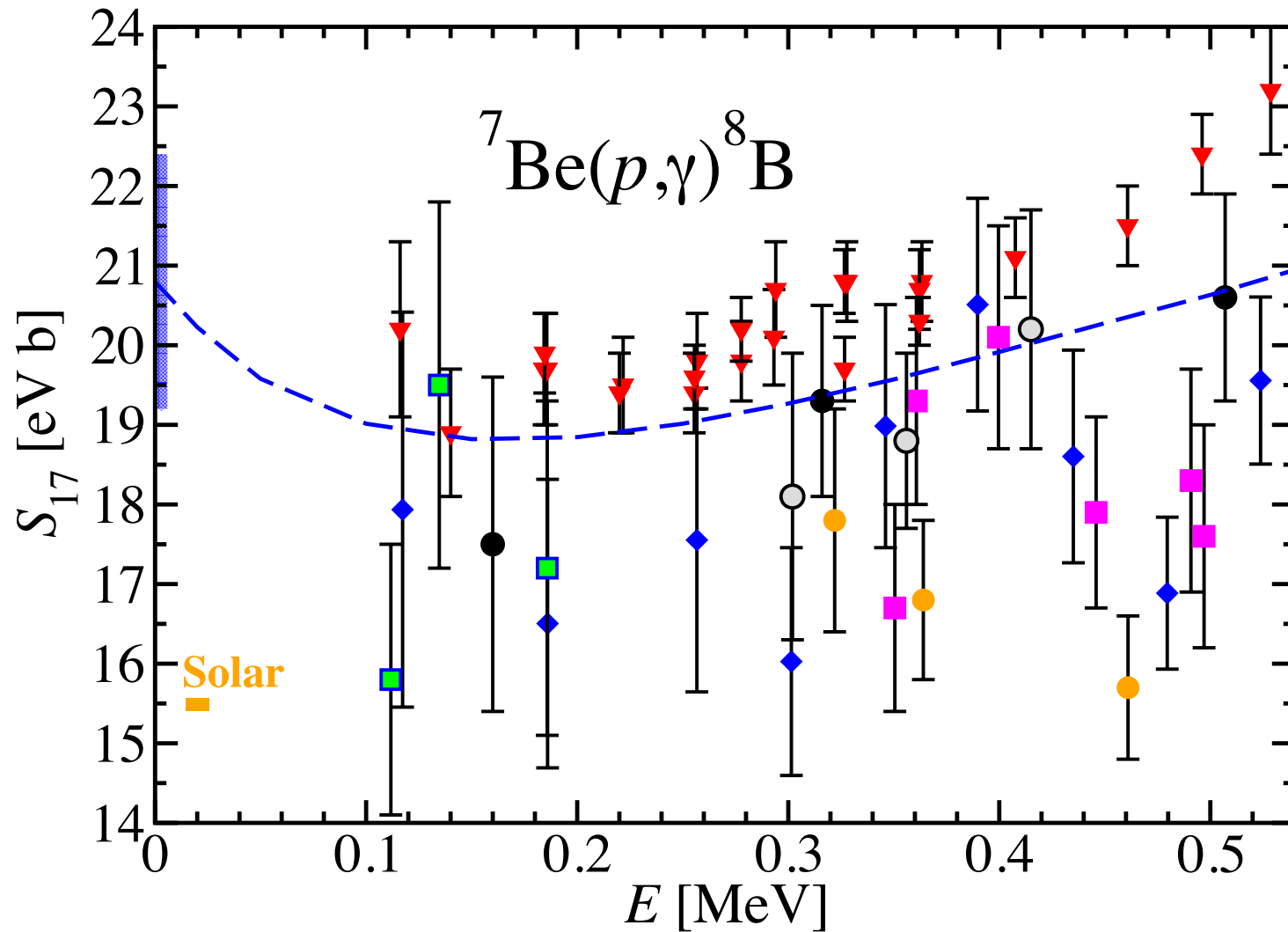
Neutrino  
oscillations  
2015 Noble Prize  
in Physics



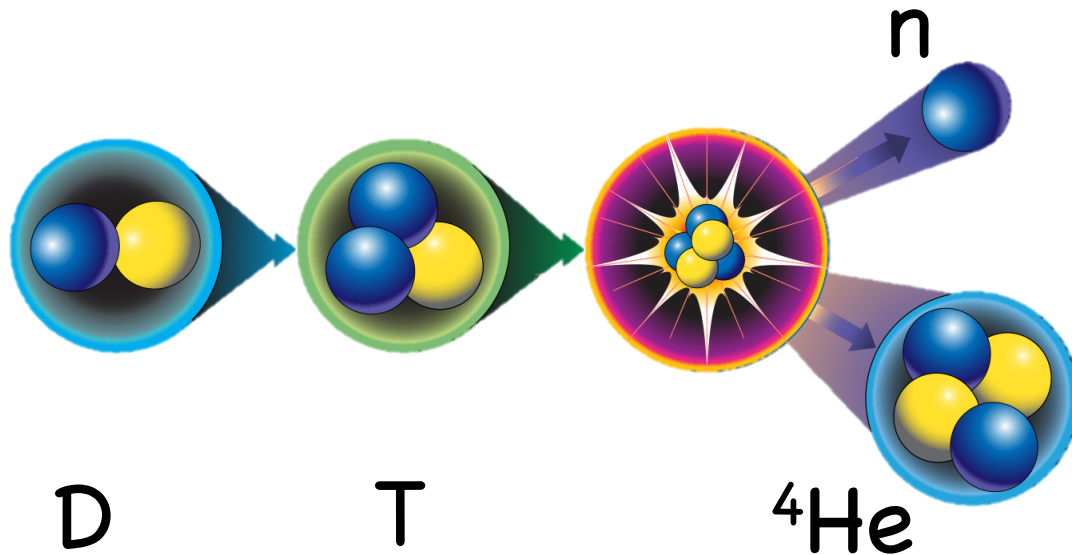
# Uncertainties in solar fusion S-factors



# Uncertainties in solar fusion S-factors



# Fusion energy generation



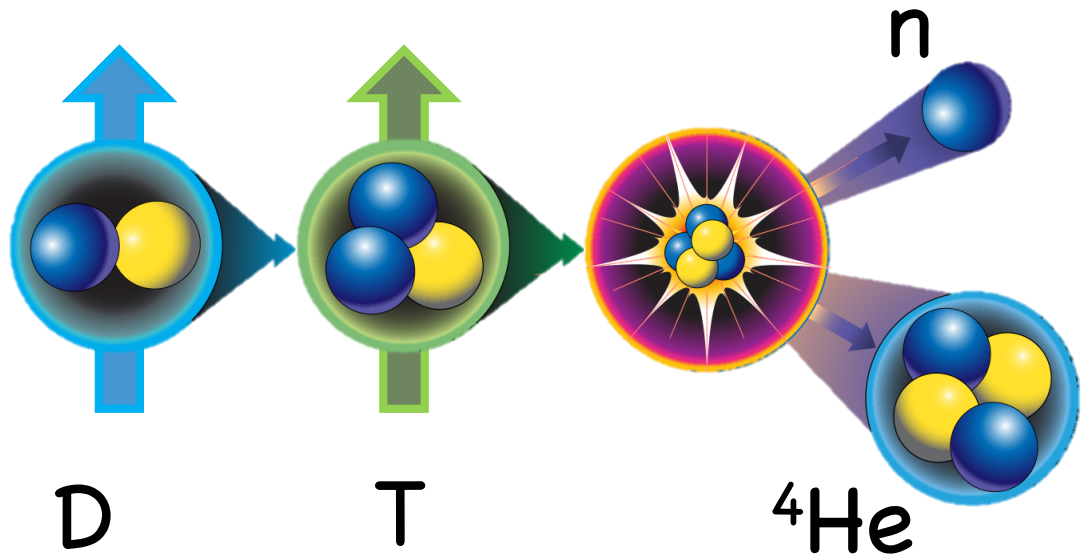
Symbol	BE (MeV)
$^4\text{He}$	28.30
$^3\text{H}$ or T	- 8.48
$^2\text{H}$ or D	- 2.22

**= +17.6 !**

- Laser confinement experiments
- Magnetic confinement experiments (ITER)



# Fusion energy generation



Symbol	BE (MeV)
$^4\text{He}$	28.30
$^3\text{H}$ or T	- 8.48
$^2\text{H}$ or D	- 2.22

= +17.6 !

- By perfectly aligning the spins of D and T estimated 50% enhancement of reaction rate
- How does the rate depend on polarization?

# Summary

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- Light nuclei are the building blocks of life and the universe as we know it
- Ongoing attempts to harness energy from thermonuclear fusion reactions
- Fusion reactions are extremely difficult to measure at stellar energies
- Predictive theory of fusion reactions needed to help extrapolate down to stellar energies

# Questions

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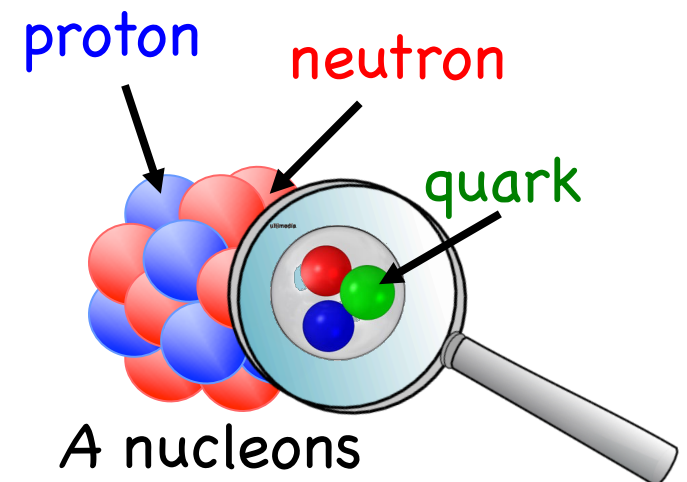
- Do you have any questions on this section?
- Question for you:
  - How much energy is released from the fusion of two  $^2\text{H}$  nuclei?
- Form a group of 2 or 3 people and take a couple of minutes to discuss ...

How can we learn  
about the basic  
nuclear interactions?

# Can we accurately explain ...

---

- ... how stable nuclei and rare isotopes are put together from the neutron and proton constituents?
- In terms of:
  - a) The laws of quantum mechanics
  - b) The underlying theory of the strong force (quantum chromodynamics)



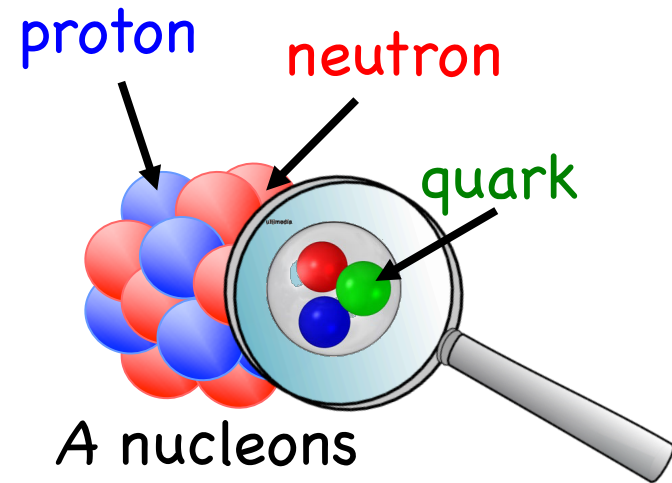
# The problem

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How do we describe these  $A$ -nucleon wave functions?

$$H\Psi = E\Psi$$

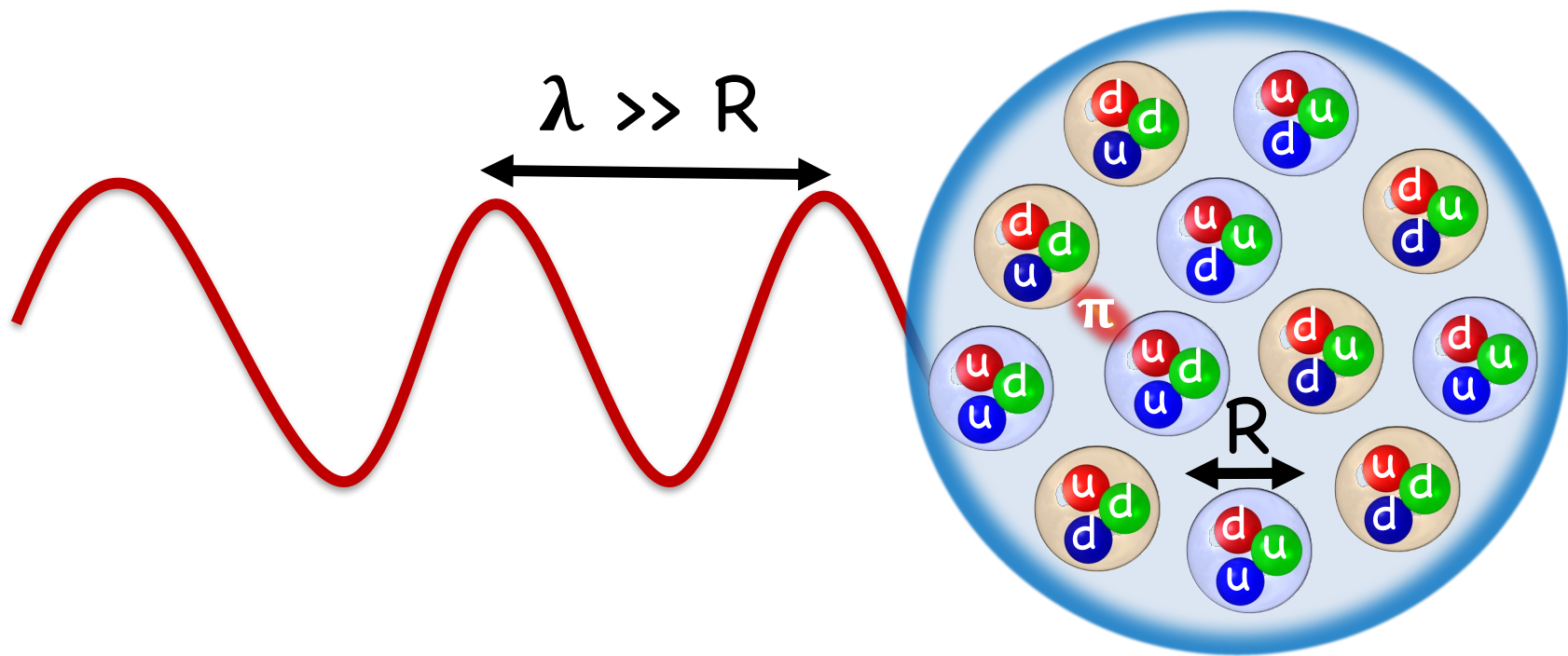
How do we describe the interactions among nucleons in this  $A$ -nucleon Hamiltonian?



How to describe the  
interactions among nucleons?

# Separation of scales

- At low energy short-distance physics is not resolved



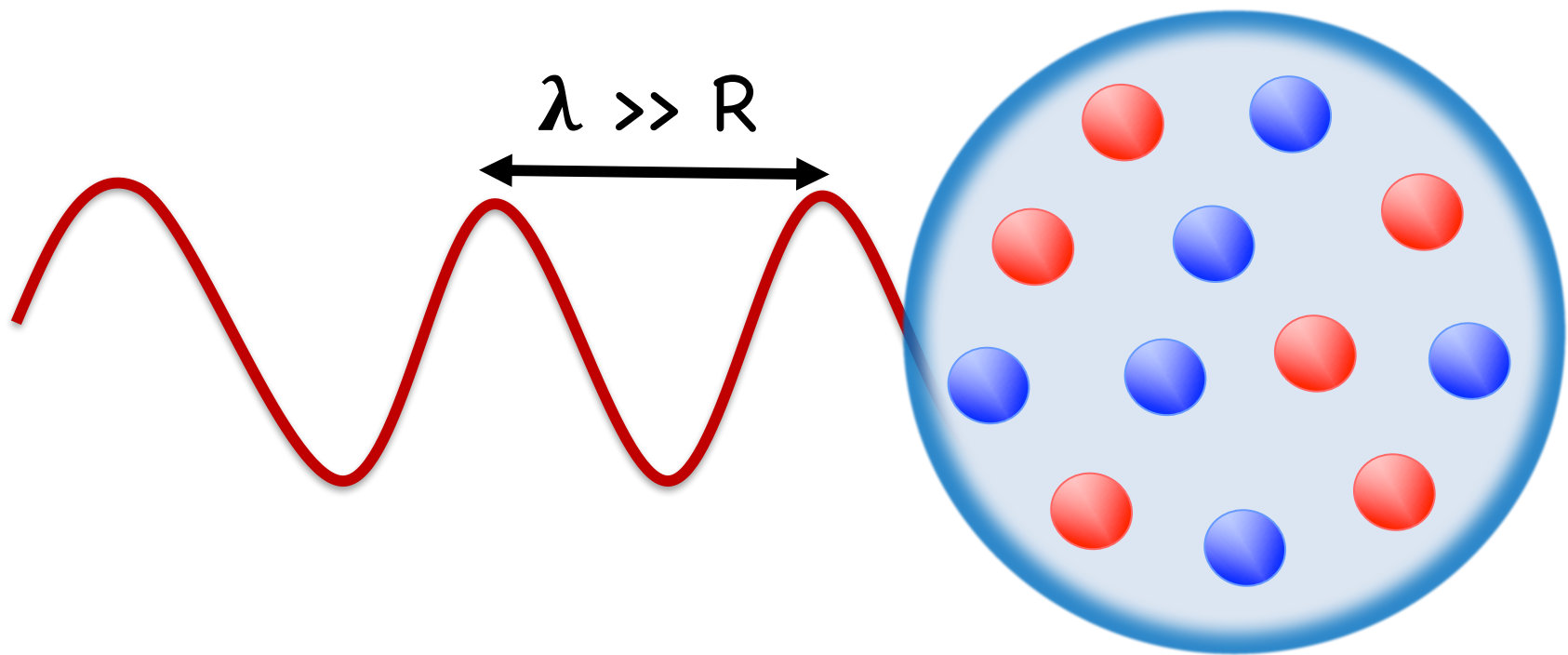
$$1/\lambda = Q \ll \Lambda = 1/R$$



# Separation of scales

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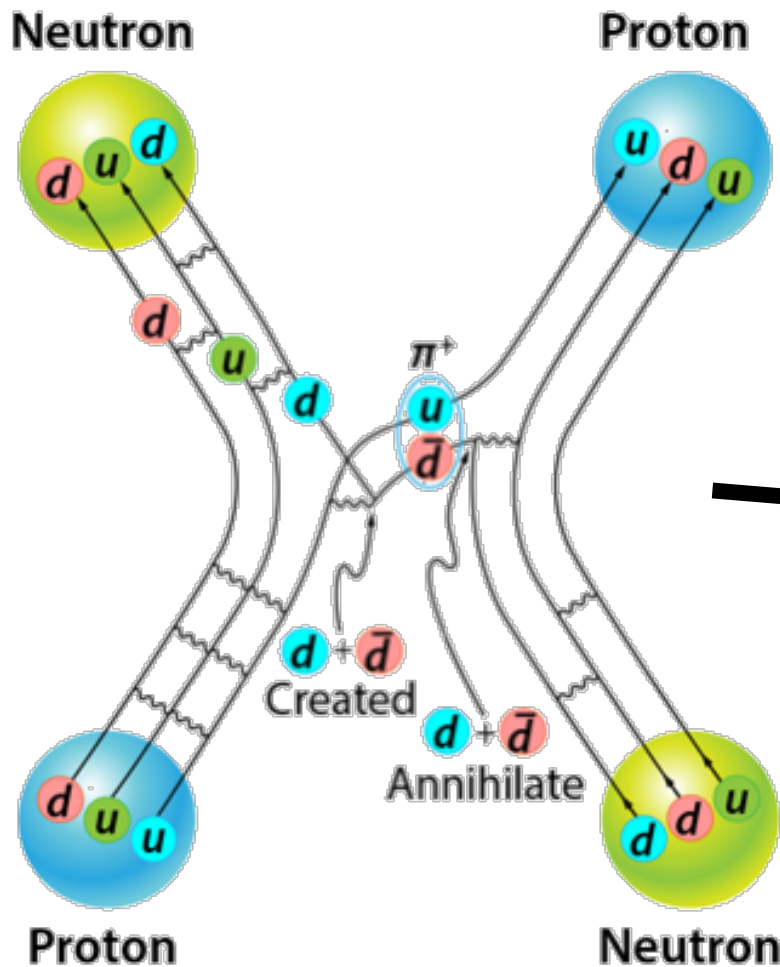
- At low energy short-distance physics is not resolved



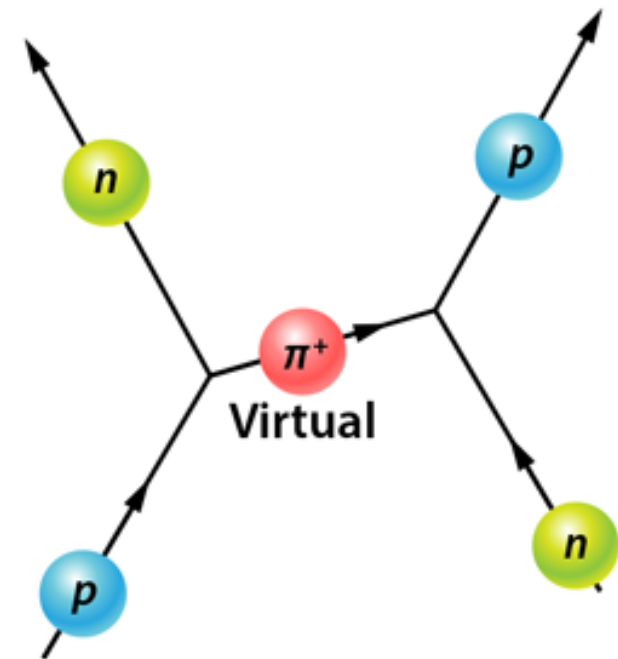
$$1/\lambda = Q \ll \Lambda = 1/R$$

# Nucleon-nucleon interaction

Quantum Chromodynamics



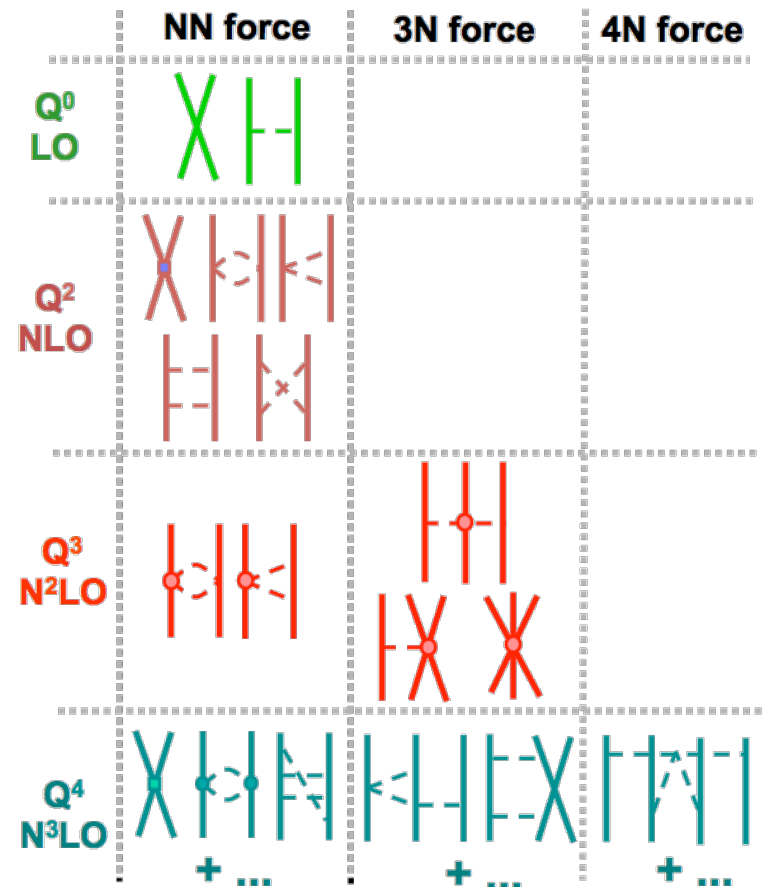
Chiral Effective Field Theory



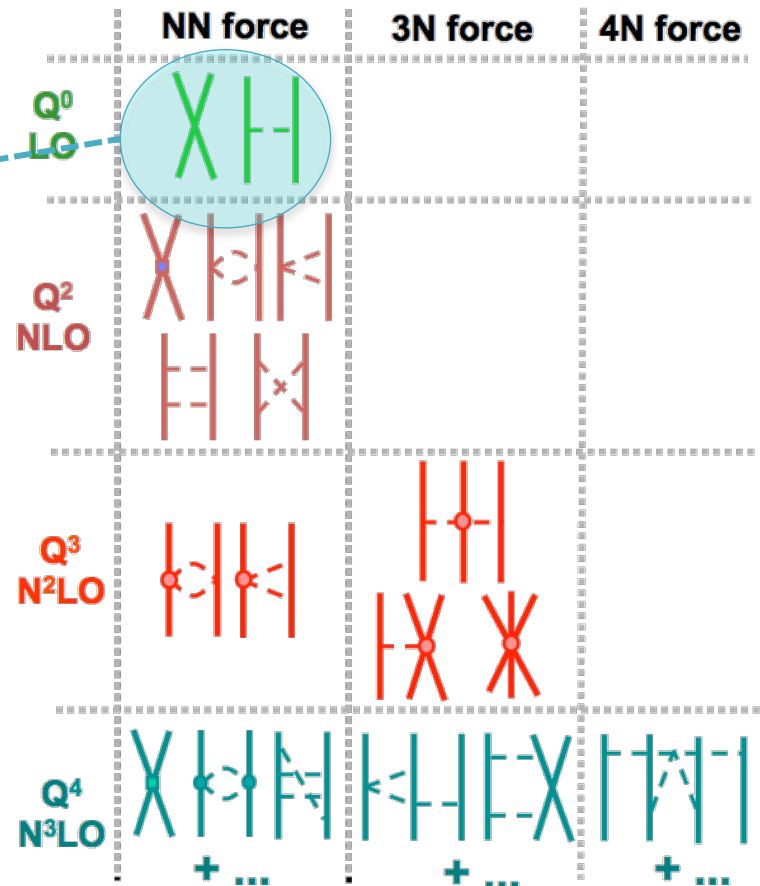
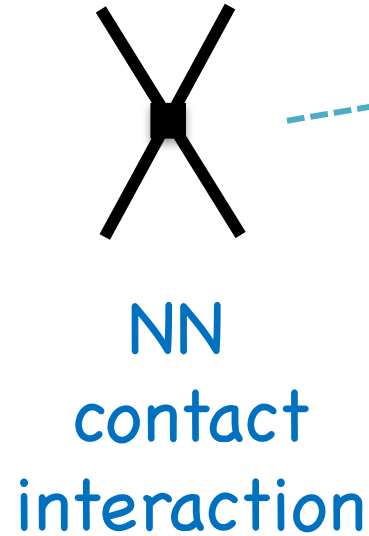
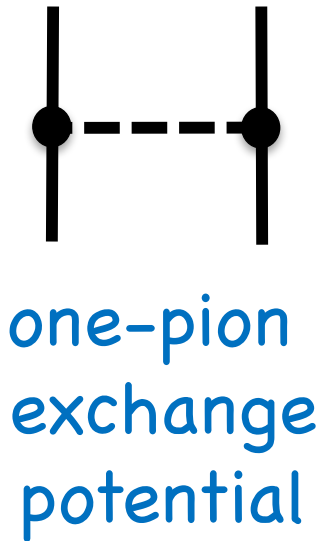
# Chiral effective field theory has transformed the way we think about and treat nuclear forces

Links the nuclear forces to the fundamental theory of quantum chromodynamics (QCD)

- organization in systematically improvable expansion:  $(Q/\Lambda)^\nu$
- empirically constrained parameters capture unresolved short-distance physics

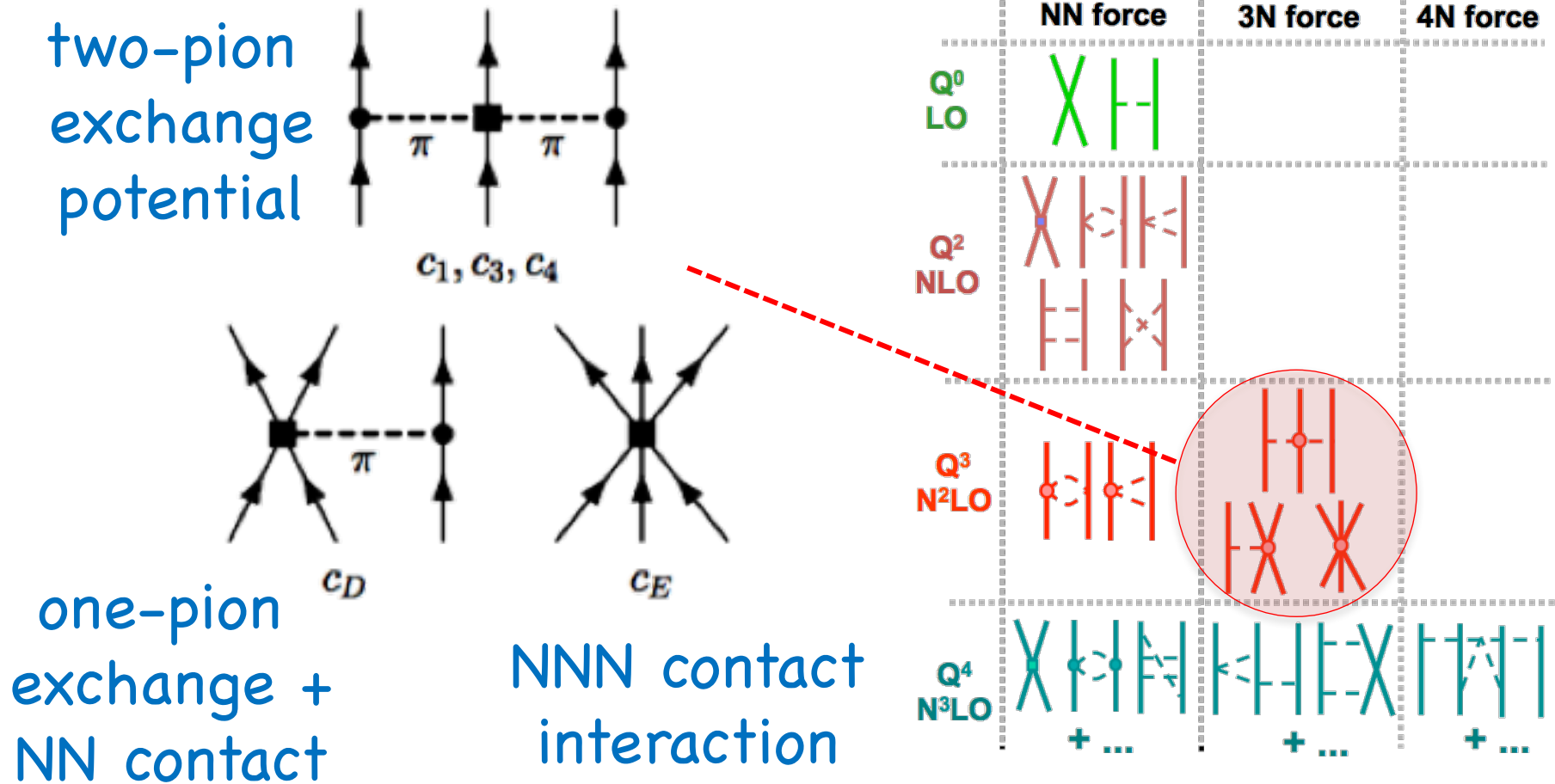


# At leading order long-range NN interaction is usual one-pion exchange



Worked out by Van Kolck, Keiser, Meissner, Epelbaum, Machleidt, ...

# Three-nucleon forces appear at N<sup>2</sup>LO

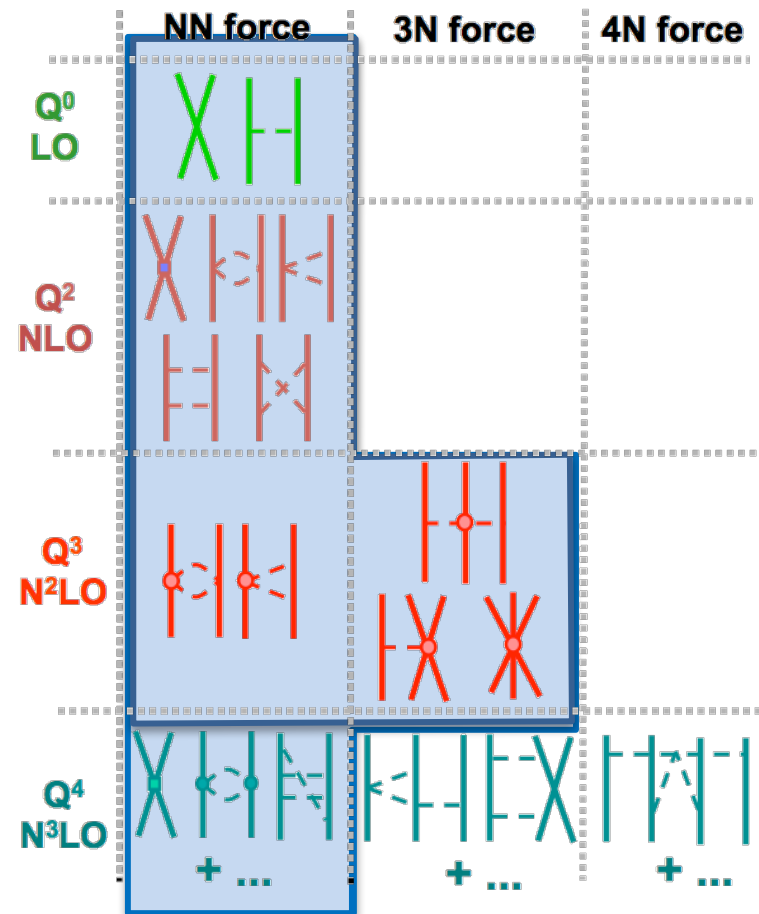


Worked out by Van Kolck, Keiser, Meissner, Epelbaum, Machleidt, ...

# How to best implement the theory and constrain it is an active topic or research

## Nomenclature/Parameterizations:

- **NN**: potential at  $N^3LO$ , 500 MeV cutoff (by Entem & Machleidt)
- **NN+3N(500)**: NN plus 3N force at  $N^2LO$ , 500 MeV cutoff (local form by Navrátil)
- **NN+3N(400)**: NN plus 3N force at  $N^2LO$ , 400 MeV cutoff (local form by Navrátil)
- **$N^2LO_{sat}$**  : NN+3N at  $N^2LO$ , fitted simultaneously (by Ekström et al.)
- ...



Worked out by Van Kolck, Keiser, Meissner, Epelbaum, Machleidt, ...

How to solve the  
Schrödinger equation?

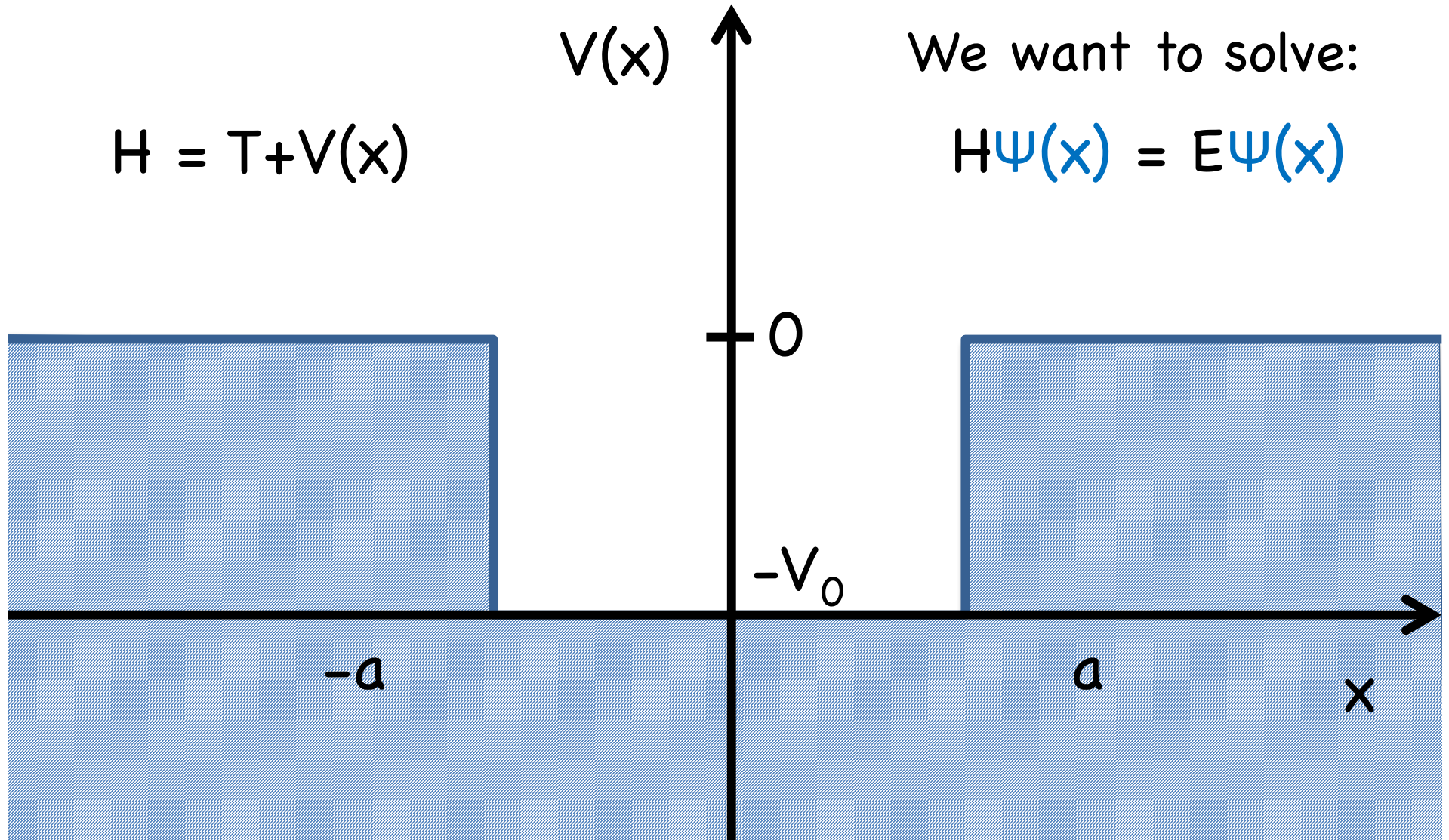
# Well-known example: one particle in 1D, finite square-well potential

---

$$H = T + V(x)$$

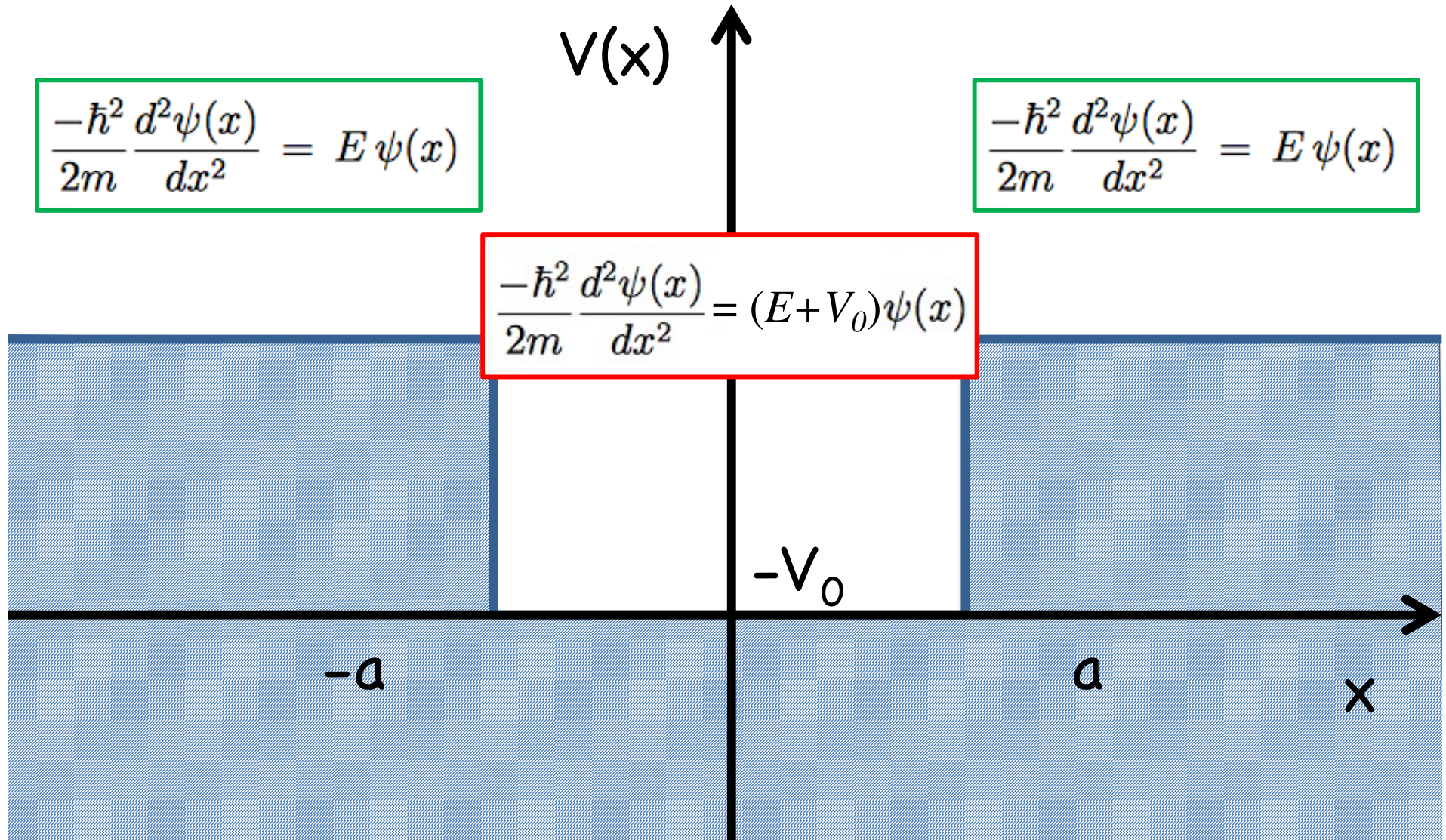
We want to solve:

$$H\Psi(x) = E\Psi(x)$$





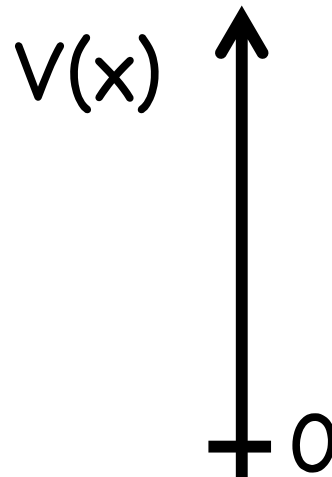
# Well-known example: one particle in 1D, finite square-well potential



# 1D finite square-well potential: $E < 0$

$$k = \frac{\sqrt{2m|E|}}{\hbar}$$

$$\alpha = \frac{\sqrt{2m(V_0 - |E|)}}{\hbar}$$



Solution by requiring continuity of  $\Psi(x)$  and  $\Psi'(x)$  at the borders ( $a$  and  $-a$ )

$$\psi(x) = Ce^{kx}$$

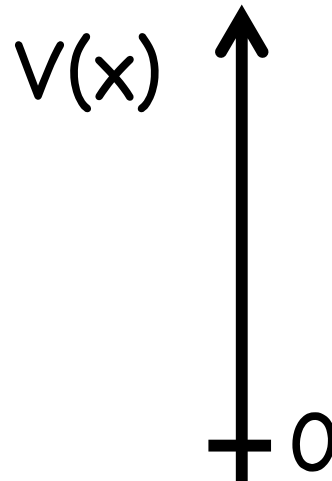
$$\psi(x) = Ae^{-i\alpha x} + Be^{i\alpha x}$$

$$\psi(x) = Ce^{-kx}$$

# 1D finite square-well potential: $E > 0$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\alpha = \frac{\sqrt{2m(V_0 + E)}}{\hbar}$$



Solution by requiring continuity of  $\Psi(x)$  and  $\Psi'(x)$  at the borders ( $a$  and  $-a$ )

$$\psi(x) = Ce^{ikx}$$

$$\psi(x) = Ae^{-i\alpha x} + Be^{i\alpha x}$$

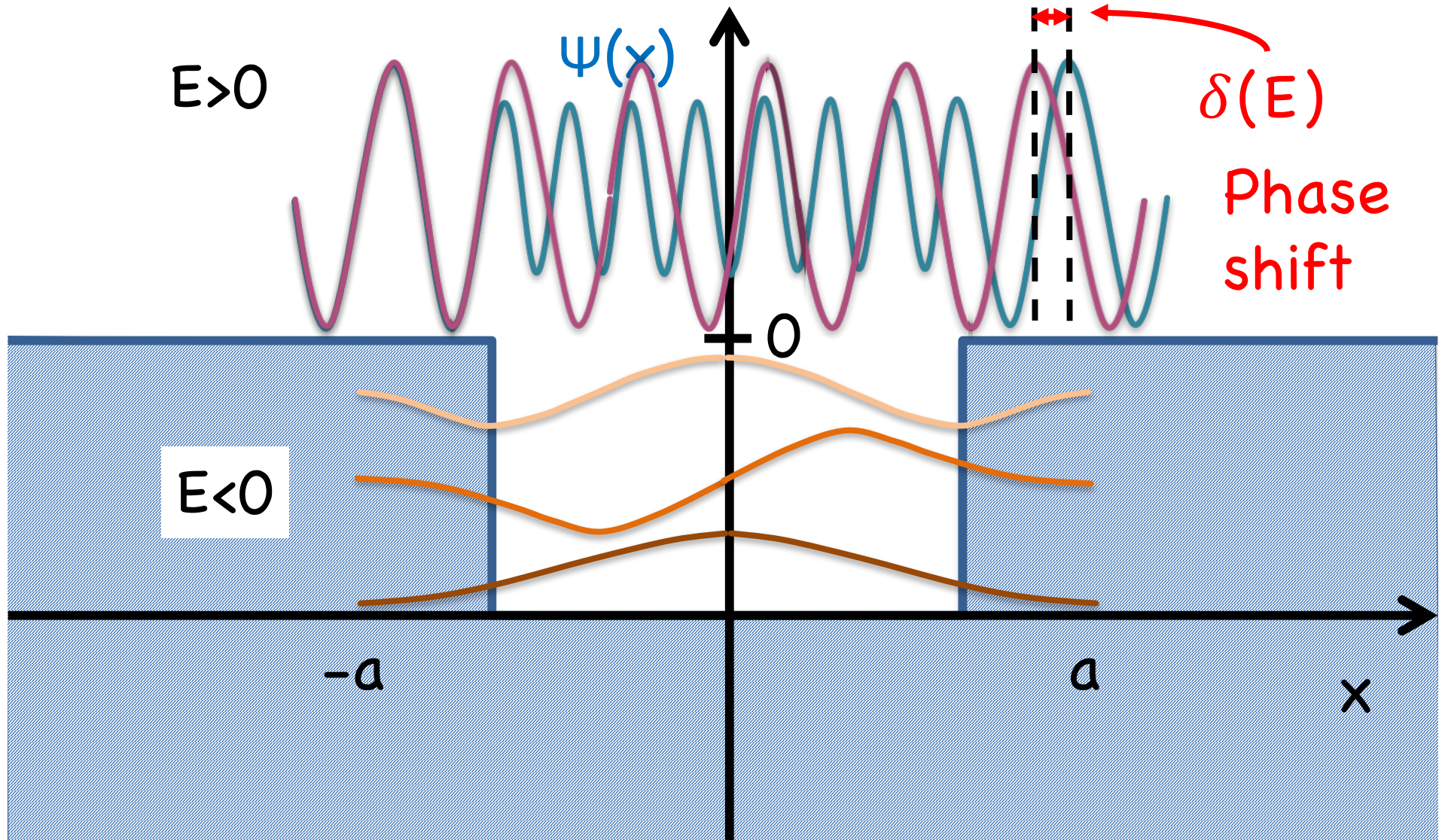
$$\psi(x) = Ce^{-ikx}$$

$-a$

$a$

$x$

# 1D finite square-well potential: solutions

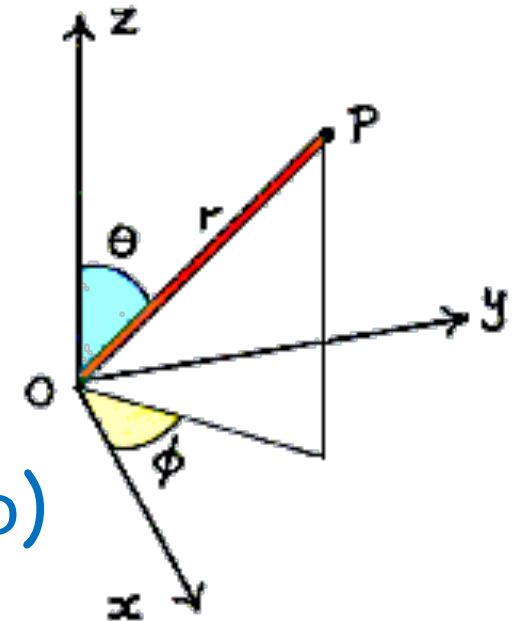


# One particle in 3D more complicated, can be solved analytically in some case

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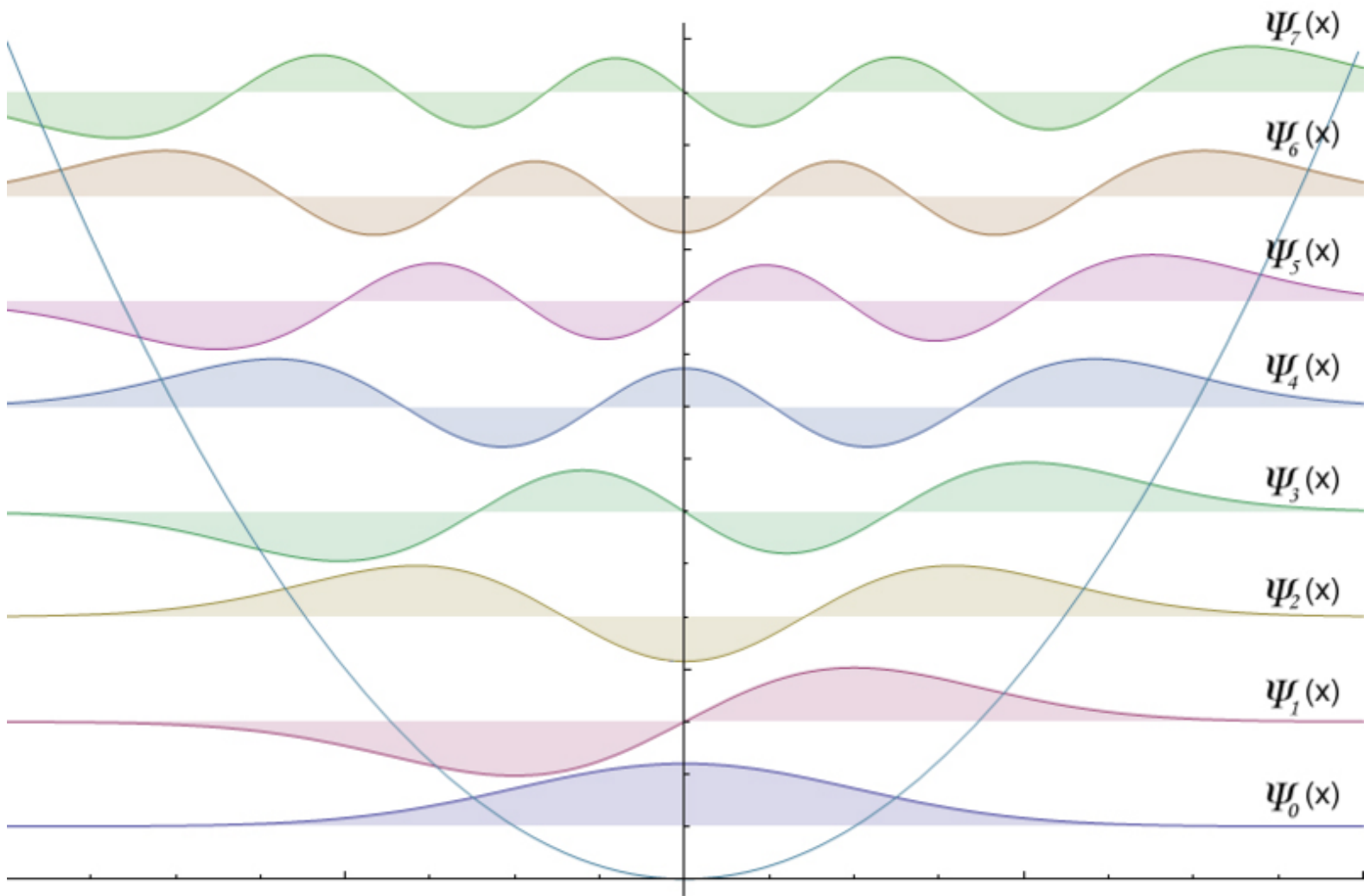
- Particle in spherically symmetric potential
  - Spherical ‘square-well’ potential
  - Harmonic Oscillator potential
  - Hydrogen-like atoms
  - ...

$$\Psi(\mathbf{r}) = R(r) Y_{\ell m}(\theta, \phi)$$



- Reduce to 1D problem using spherical coordinates, spherical harmonics

# Harmonic oscillator potential



# Two-nucleon problem

---

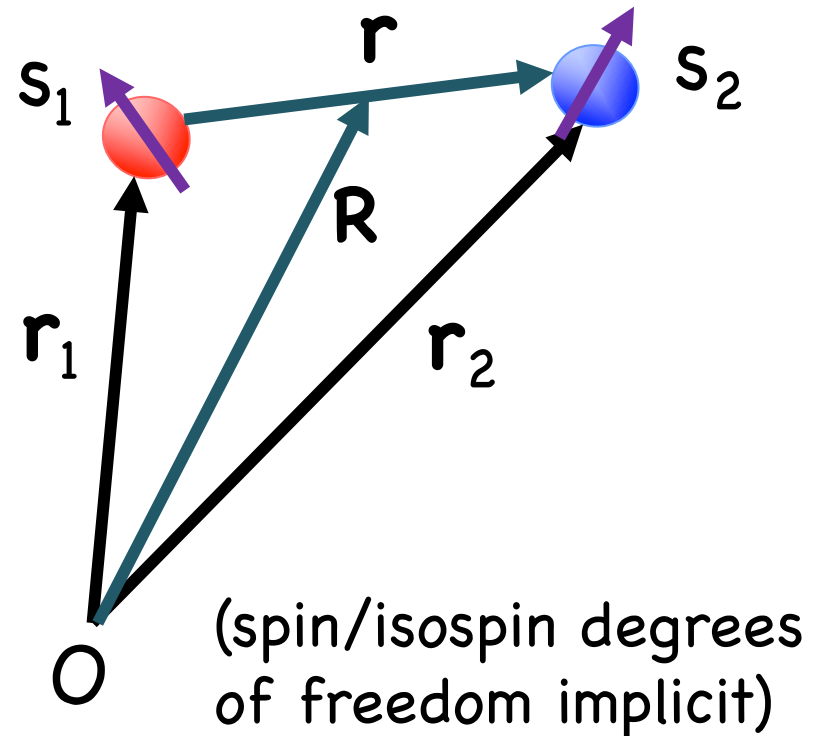
$$H^{(2)} = T_1 + T_2 + V(|\mathbf{r}_1 - \mathbf{r}_2|)$$

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

$$\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$$

$$\mathbf{k} = (\mathbf{p}_1 - \mathbf{p}_2)/2$$

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$$



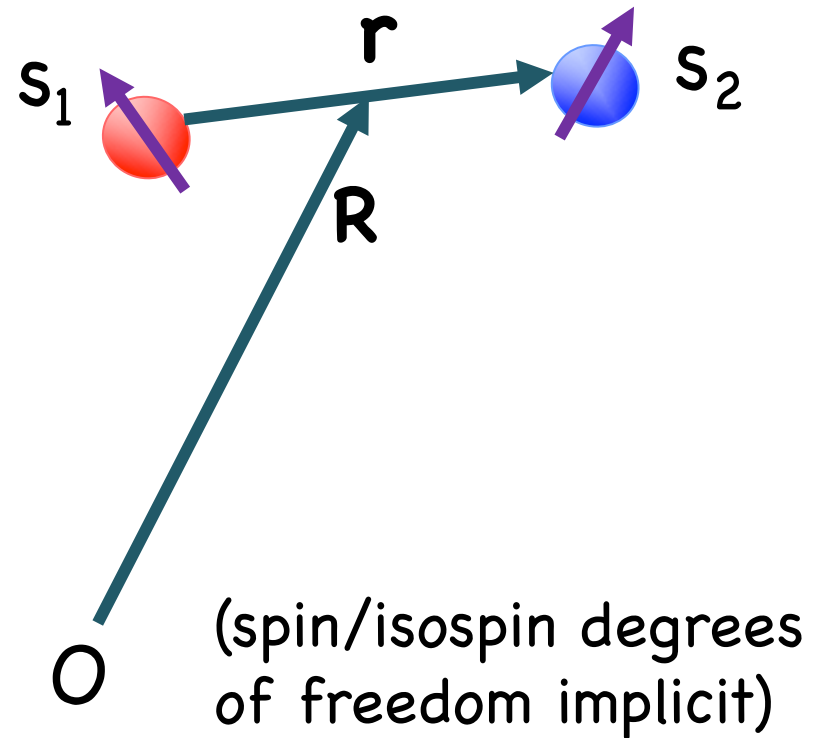
# Two-nucleon problem

---

$$\begin{aligned} H^{(2)} &= T_{\text{cm}} + T_k + V(r) \\ &= T_{\text{cm}} + H_{\text{int}} \end{aligned}$$



$$\Psi(\mathbf{r}, \mathbf{R}) = e^{-i\mathbf{P}\mathbf{R}} \psi_{\text{int}}(\mathbf{r})$$





# Two-nucleon problem

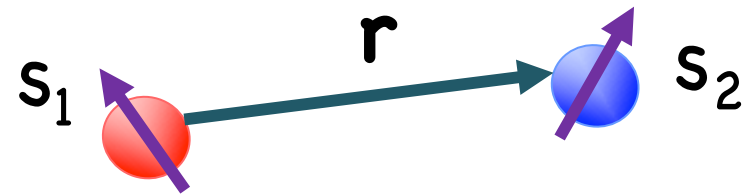
- Reduce to one-body 3D problem for the intrinsic motion ...

$$H_{\text{int}} \Psi_{\text{int}}(\mathbf{r}) = E \Psi_{\text{int}}(\mathbf{r})$$

- ... and to 1D problem

$$\Psi_{\text{int}}(\mathbf{r}) = \sum_{\kappa} C_{\kappa} R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \chi_{S\tau}(1,2) \chi_{T\tau}(1,2)$$

all quantum numbers  $\nearrow$   $\kappa$       radial      orbital angular      spin      isospin



$$\mathbf{S} = 1/2 + 1/2 = 0, 1$$

$$\mathbf{T} = 1/2 + 1/2 = 0, 1$$

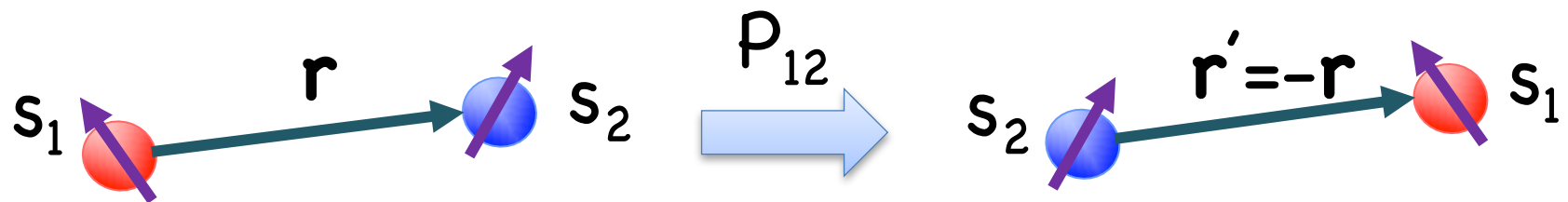
# Two-nucleon problem

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- Nucleons are identical particles
- Spin statistic theorem:
  - Bosons = integer spin  $\rightarrow P_{12}\psi = \psi$  (symmetric)
  - Fermions = half-integer spin  $\rightarrow P_{12}\psi = -\psi$   
(antisymmetric)

# Two-nucleon problem

---



$$R_{n\ell}(r) Y_{\ell m}(\theta, \phi)$$

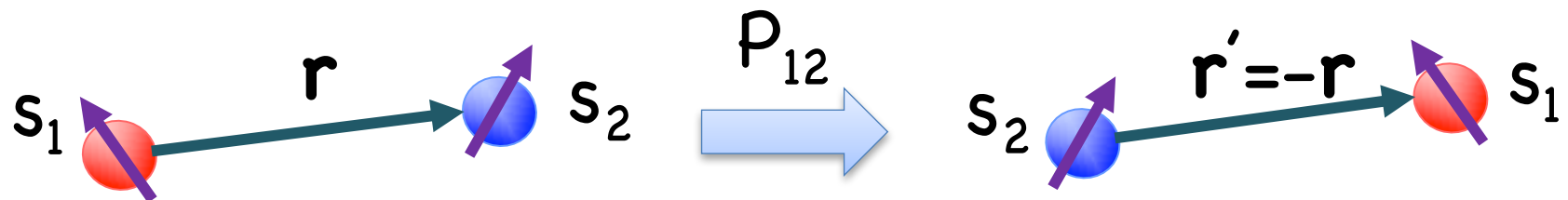
$$\chi_{su}(1,2) \chi_{T\tau}(1,2)$$

$$R_{n\ell}(r) Y_{\ell m}(\pi - \theta, 2\pi + \phi)$$

$$\chi_{su}(2,1) \chi_{T\tau}(2,1)$$

# Two-nucleon problem

---



$$R_{n\ell}(r) Y_{\ell m}(\theta, \phi)$$

$$\chi_{S_U}(1,2) \chi_{T_T}(1,2)$$

$$(-1)^{\ell+S+T} R_{n\ell}(r) Y_{\ell m}(\pi, \phi)$$

$$\chi_{S_U}(1,2) \chi_{T_T}(1,2)$$

Only the components for which  $\ell+S+T$  is odd are physical two-nucleon configurations

# Two-nucleon problem: To summarize

---

- Reduces to 1D 1-body problem by
  - 1) Moving to relative coordinates
  - 2) Using expansion in spherical harmonics
- Solutions have to be antisymmetric under nucleon exchange (Pauli exclusion principle)
- Can be solved analytically only in a few cases (e.g., harmonic oscillator potential)
- With chiral forces need to solve numerically

# Questions

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- Do you have any questions?
- Question for you:
  - What are the physical two-nucleon channels?

# Some physical two-nucleon channels

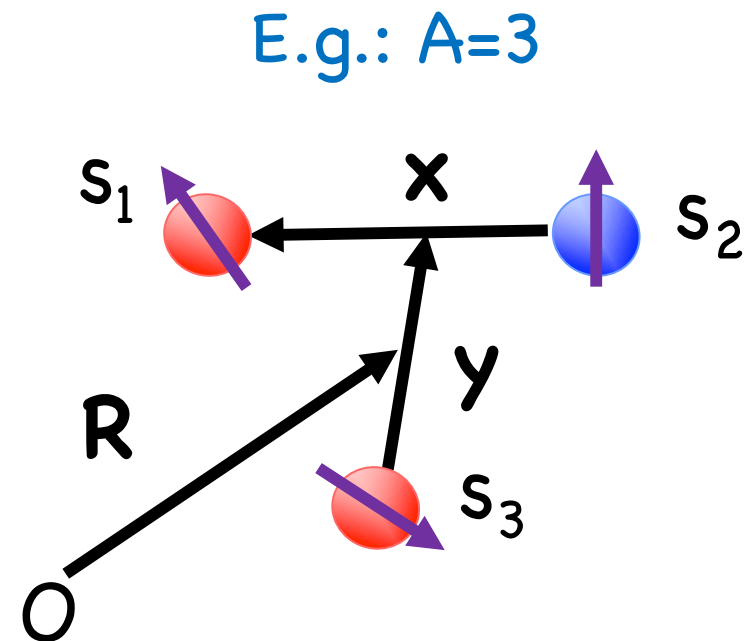
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- ~~$\ell = 0, S = 0, J = 0, T = 0?$~~
- $\ell = 0, S = 0, J = 0, T = 1?$
- $\ell = 0, S = 1, J = 1, T = 0?$
- ~~$\ell = 0, S = 1, J = 1, T = 1?$~~
- $\ell = 1, S = 0, J = 1, T = 0?$
- ~~$\ell = 1, S = 0, J = 1, T = 1?$~~
- ...

# Few-nucleon problem: $A = 3, 4, 5 \dots$

---

- Use 'Jacobi' coordinates (generalization of 2-body relative coordinates)
- Use expansion in hyperspherical harmonics (generalization of 1D spherical harmonics)
- Hard to antisymmetrize!

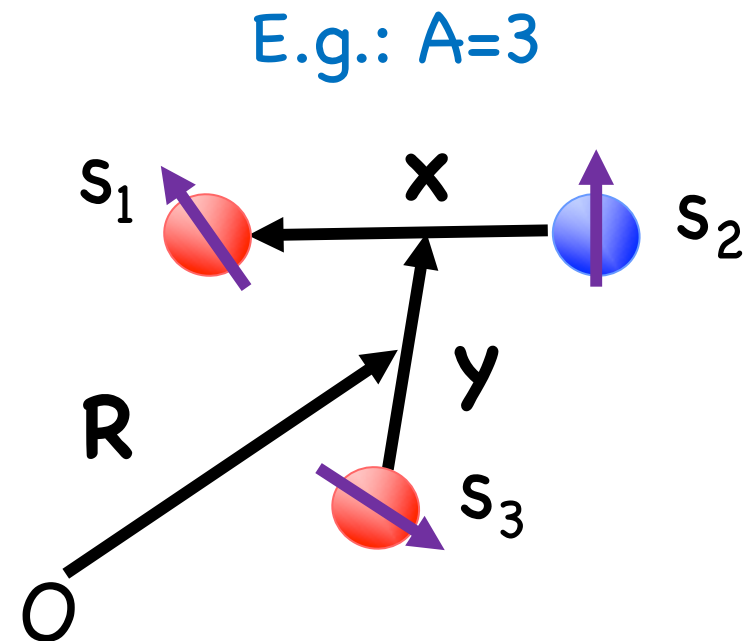




# Few-nucleon problem: $A = 3, 4, (5), 6 \dots$

Main examples:

- Faddeev equations ( $A=3$ )
- Faddeev-Yacubovsky ( $A=4, 5^*$ ), Alt-Grassberger-Sandhas equations ( $A=4$ )
- Jacobi-coordinate no-core shell model ( $A = 3, 4$ )
- Hyperspherical harmonics expansions ( $A = 3, 4, 6$ )

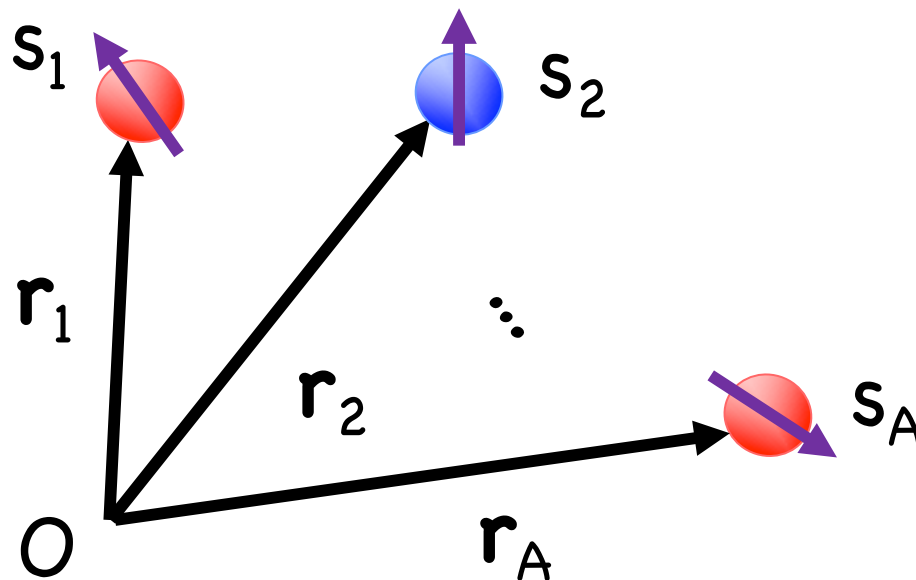


\* New development!

# A-nucleon problem

---

$$H^{(A)} = \sum_{i=1}^A T_i + \sum_{i < j=1}^A V^{NN}(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_{i < j < k=1}^A V_{ijk}^{3N}$$



# A-nucleon problem

---

- A position coordinates ( $A-1$  without C.M.)
- A spin coordinates
- A isospin coordinates
- The solution has to be antisymmetric under exchange of any two nucleons
- Way to complicated to solve as before!

What to do???

... search under the lamp post!



*"I'm searching for my keys."*

# We know how to solve the independent-particle problem

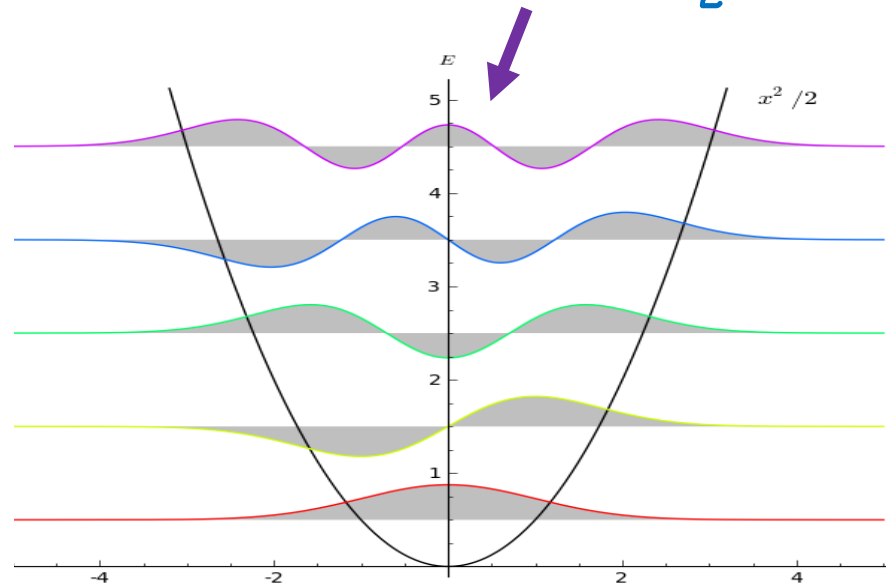
$$\tilde{H}^{(A)} = \sum_{i=1}^A T_i + U(r_i) = \sum_{i=1}^A h_i$$

Single-particle Hamiltonian

1) Solve single-particle problem:

e.g.:  $U(r) = \frac{1}{2}m\Omega^2 r^2$

$$h \varphi_n(\mathbf{r}) = \varepsilon_n \varphi_n(\mathbf{r})$$



# We know how to solve the independent-particle problem

---

2) The antisymmetric A-nucleon solutions can be build as

$$\Phi_k = \frac{1}{\sqrt{A!}} \det \begin{pmatrix} \varphi_{k1}(\mathbf{r}_1) & \varphi_{k1}(\mathbf{r}_2) & \dots & \varphi_{k1}(\mathbf{r}_A) \\ \varphi_{k2}(\mathbf{r}_1) & \varphi_{k2}(\mathbf{r}_2) & \dots & \varphi_{k2}(\mathbf{r}_A) \\ \vdots & \vdots & & \vdots \\ \varphi_{kA}(\mathbf{r}_1) & \varphi_{kA}(\mathbf{r}_2) & \dots & \varphi_{kA}(\mathbf{r}_A) \end{pmatrix}$$

We have that:

$$H^{(A)} \Phi_k = E_k \Phi_k \quad \text{with} \quad E_k = \sum_{i=1}^A \varepsilon_{ki} d_{ki}$$

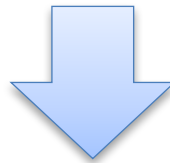
Degeneracy  


# What about our original A-nucleon problem?

---

- 3) Use the independent-particle model solutions as 'basis states' to **build an ansatz** for the A-nucleon wave function

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = \sum_k^N c_k \Phi_k(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$$



$$(H^{(A)} - E) \Psi = 0 \Rightarrow \sum_k^N c_k (H^{(A)} - E) \Phi_k = 0$$

Maximum  
number of  
excitations

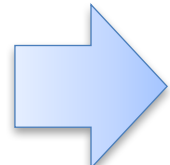
# What about our original A-nucleon problem?

---

4) Project the equation on the basis states (from the left)

$$\sum_k^N c_k \int \Phi_m^*(\mathbf{r}_1, \dots, \mathbf{r}_A) H^{(A)} \Phi_k(\mathbf{r}_1, \dots, \mathbf{r}_A) d\mathbf{r}_1 \dots d\mathbf{r}_A$$
$$= E \sum_k^N c_k \int \Phi_m^*(\mathbf{r}_1, \dots, \mathbf{r}_A) \Phi_k(\mathbf{r}_1, \dots, \mathbf{r}_A) d\mathbf{r}_1 \dots d\mathbf{r}_A$$

$\delta_{mk}$


$$\sum_k^N \mathbf{H}_{mk} c_k = E c_m$$



# What about our original A-nucleon problem?

---

The A-nucleon Schrödinger equation becomes a linear algebra eigenvalue problem

$$\mathbf{H} \mathbf{c} = E \mathbf{c} \leftarrow \text{unknown}$$

- The elements of the  $N \times N$  Hamiltonian matrix are

$$H_{mk} = \int \phi_m^*(\mathbf{r}_1, \dots, \mathbf{r}_A) H^{(A)} \phi_k(\mathbf{r}_1, \dots, \mathbf{r}_A) d\mathbf{r}_1 \dots d\mathbf{r}_A$$

- And the **unknown** expansion coefficients  $c_k$  are the elements of the eigenvector  $\mathbf{c}$

# What about our original A-nucleon problem?

---

The A-nucleon Schrödinger equation becomes a linear algebra eigenvalue problem

$$\mathbf{H} \mathbf{c} = E \mathbf{c}$$

- The elements of the  $N \times N$  Hamiltonian matrix are

$$\mathbf{H}_{mk} = \langle \Phi_m | H^{(A)} | \Phi_k \rangle$$

Short-hand notation

- And the **unknown** expansion coefficients  $c_k$  are the elements of the eigenvector  $\mathbf{c}$

# Some notes

---

- This is an ‘expansion’ technique: uses large (but finite!) expansion on A-body basis states
- Convergence to the exact result is approached (variationally) by increasing **N** (i.e., basis size)
- Antisymmetrization is trivial
  
- Did we forget about anything?

# What about the center of mass motion?

---

- In the independent-particle problem, in general the c.m. motion is mixed with intrinsic motion, giving rise to spurious effects
- Exception: harmonic oscillator (HO) potential is exactly separable

$$\tilde{H}^{(\text{HO})} = \sum_{i=1}^A T_i + \frac{1}{2} m \Omega^2 r^2$$

# What about the center of mass motion?

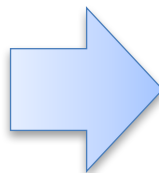
---

- In the independent-particle problem, in general the c.m. motion is mixed with intrinsic motion, giving rise to spurious effects
- Exception: harmonic oscillator (HO) potential is exactly separable

$$\tilde{H}^{(HO)} = \underbrace{T_{\text{int}} + \sum_{i < j=1}^A \frac{m\Omega^2}{2A} (\mathbf{r}_i - \mathbf{r}_j)^2}_{H_{\text{int}}} + \underbrace{T_{\text{cm}} + \frac{1}{2} Am\Omega^2 R^2}_{H_{\text{cm}}}$$

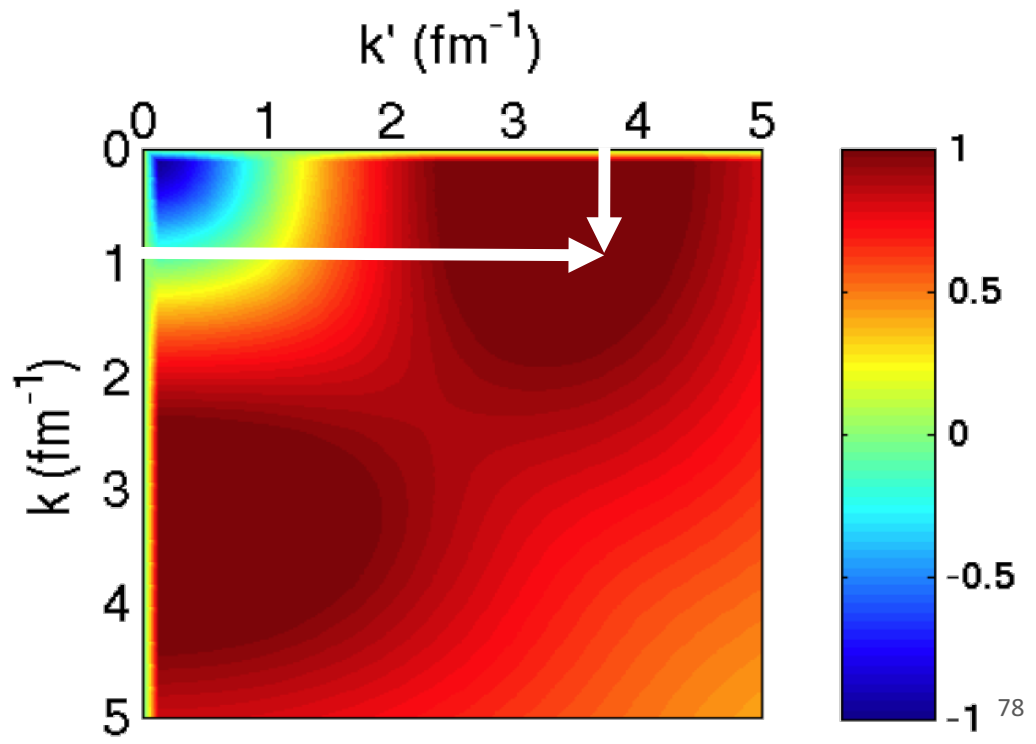
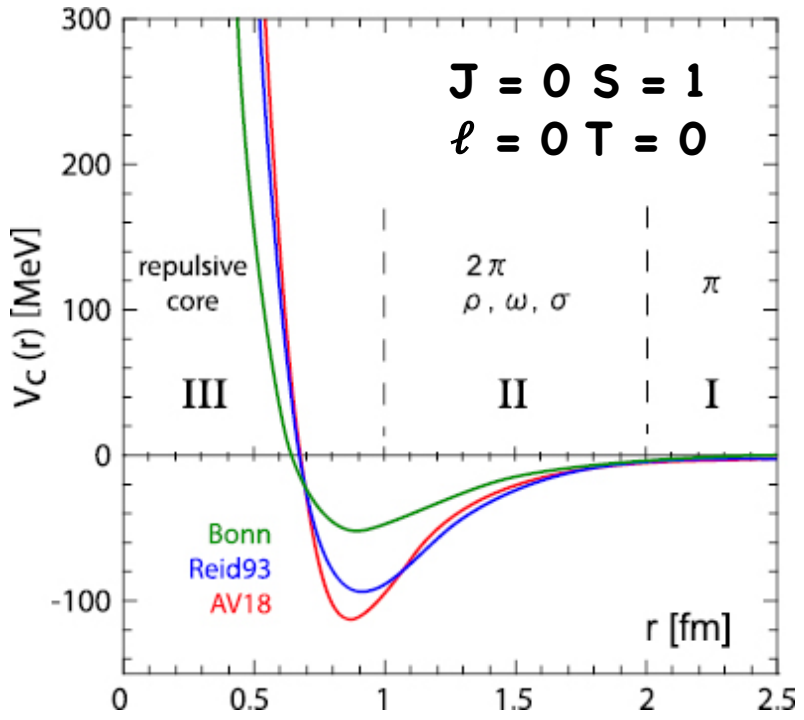
# Hard core of nuclear interaction scatters nucleons to high momenta

$V(r)$       Fourier Transform



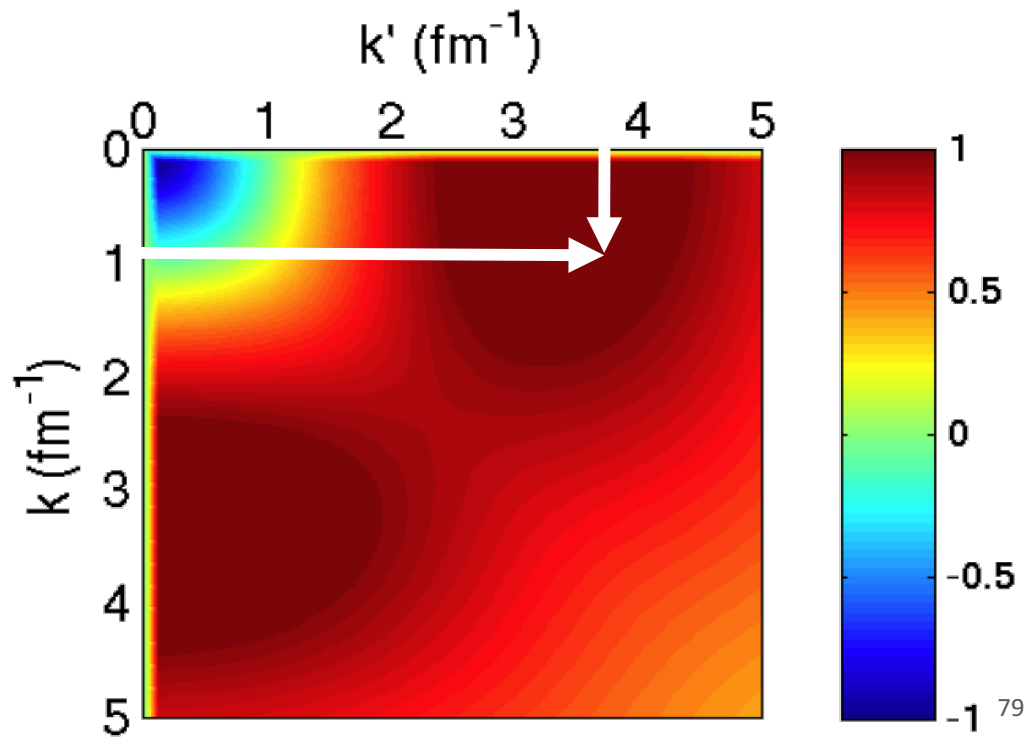
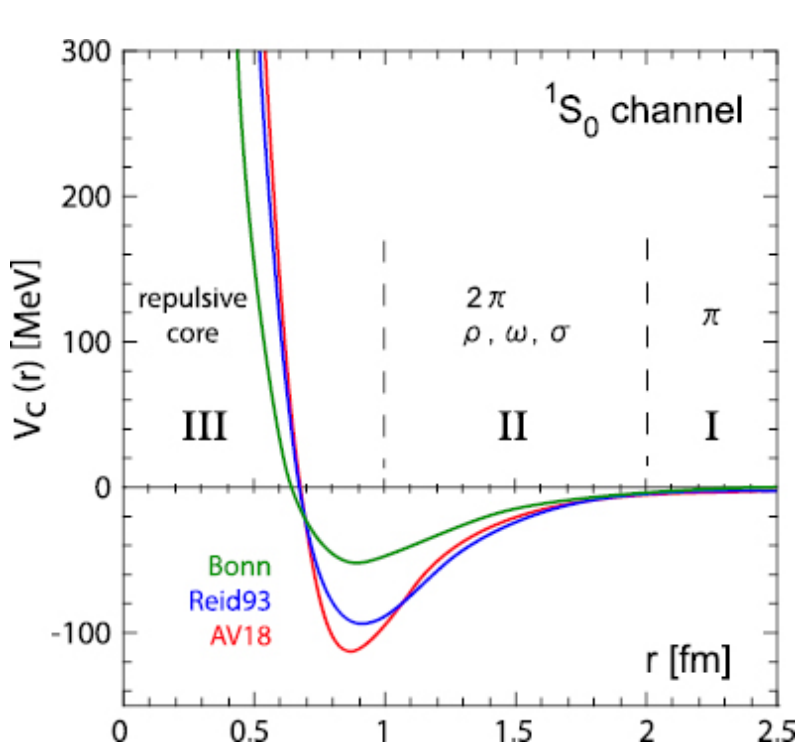
$$V_{kk'} = \int e^{ik'r} V(r) e^{-ikr} dr$$

$$= \langle k | V | k' \rangle$$



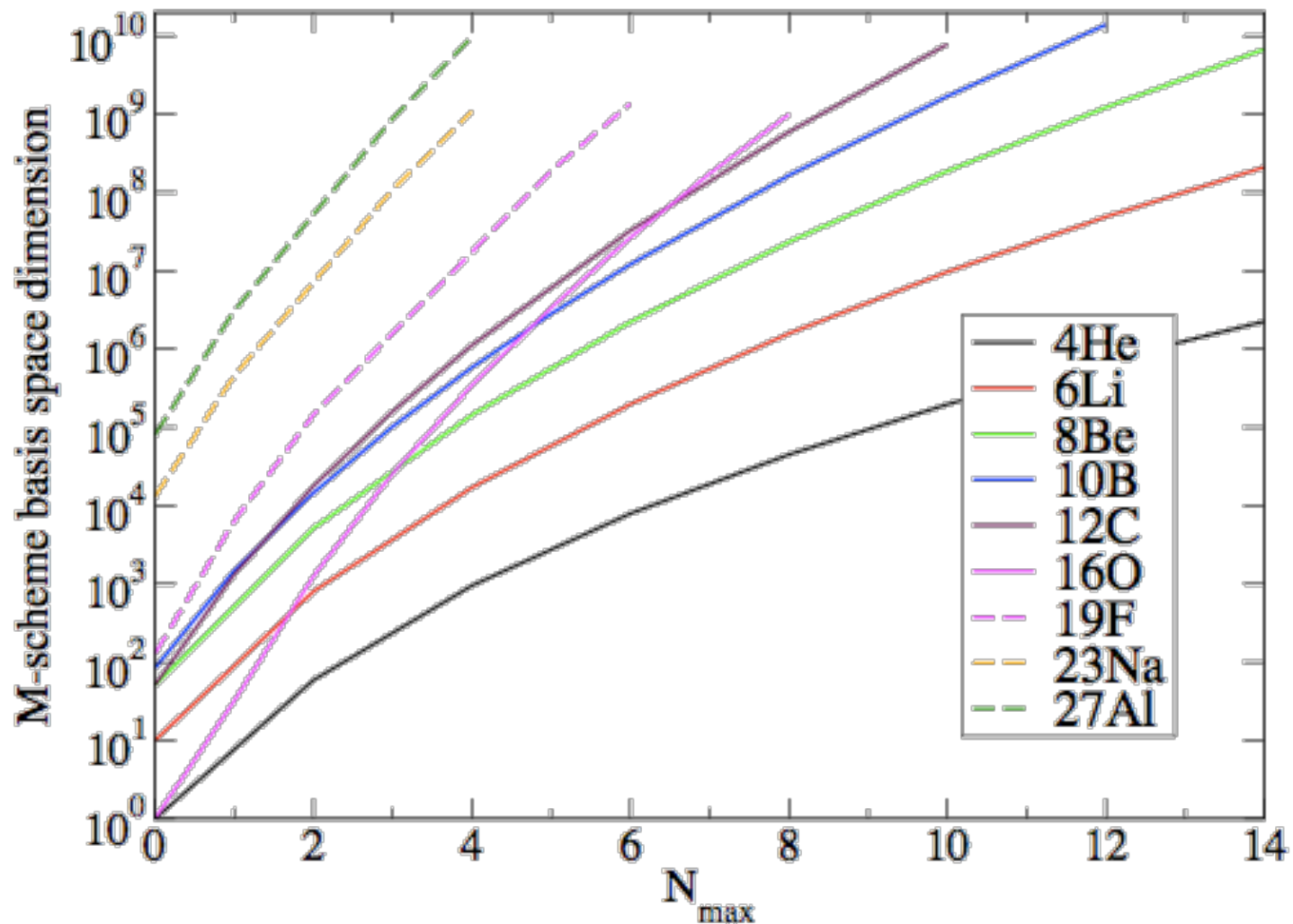
# Hard core of nuclear interaction scatters nucleons to high momenta

Very large  $N$  values (basis sizes) are required to reach convergent solution!



# Basis dimension grows rapidly with A!

Convergence can be a challenge!





# Effective interactions from unitary transformations of bare Hamiltonian

---

- Introduce unitary transformation:  $U$  ( $U^\dagger U = \mathbb{1}$ )

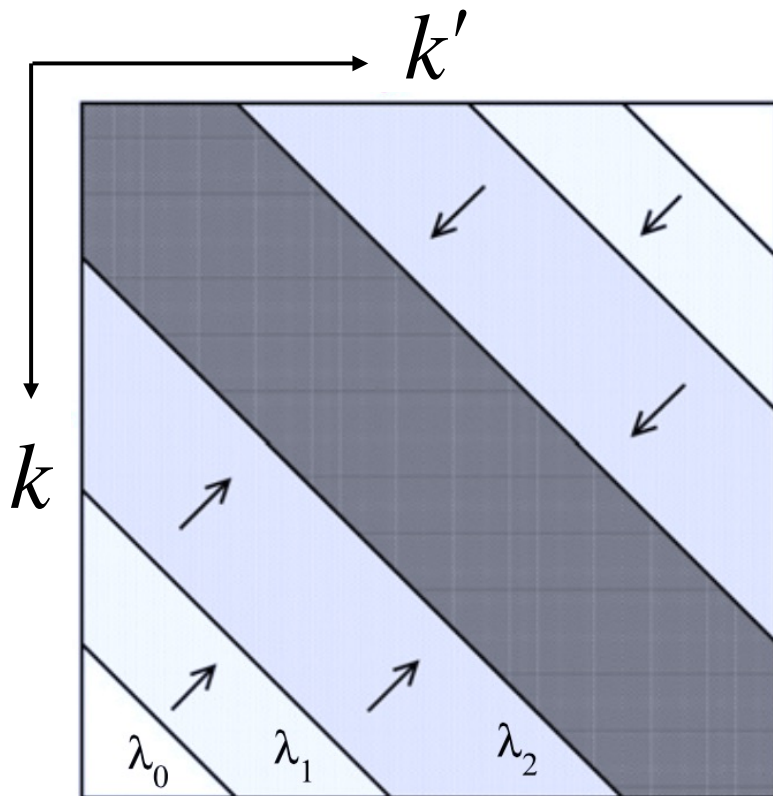
$$\begin{aligned} E &= \langle \Psi | H^{(A)} | \Psi \rangle && \begin{array}{l} \text{Bare} \\ \text{Hamiltonian,} \\ \text{wave function} \end{array} \\ &= \langle \Psi | U^\dagger H^{(A)} U | \Psi \rangle \\ &= (\langle \Psi | U^\dagger) U H^{(A)} U^\dagger (U | \Psi \rangle) \\ &= \langle \tilde{\Psi} | \tilde{H}^{(A)} | \tilde{\Psi} \rangle && \begin{array}{l} \text{Effective} \\ \text{Hamiltonian,} \\ \text{wave function} \end{array} \end{aligned}$$

# Example: Similarity renormalization group (SRG) transformation

$$\tilde{H}_\lambda = U_\lambda H U_\lambda^\dagger$$

$$\frac{d\tilde{H}_\lambda}{d\lambda} = -\frac{4}{\lambda^5} [\eta(\lambda), \tilde{H}_\lambda]$$

Flow parameter



Two-body Hamiltonian in momentum space

$$\langle k | \tilde{H}_\lambda^{(2)} | k' \rangle$$

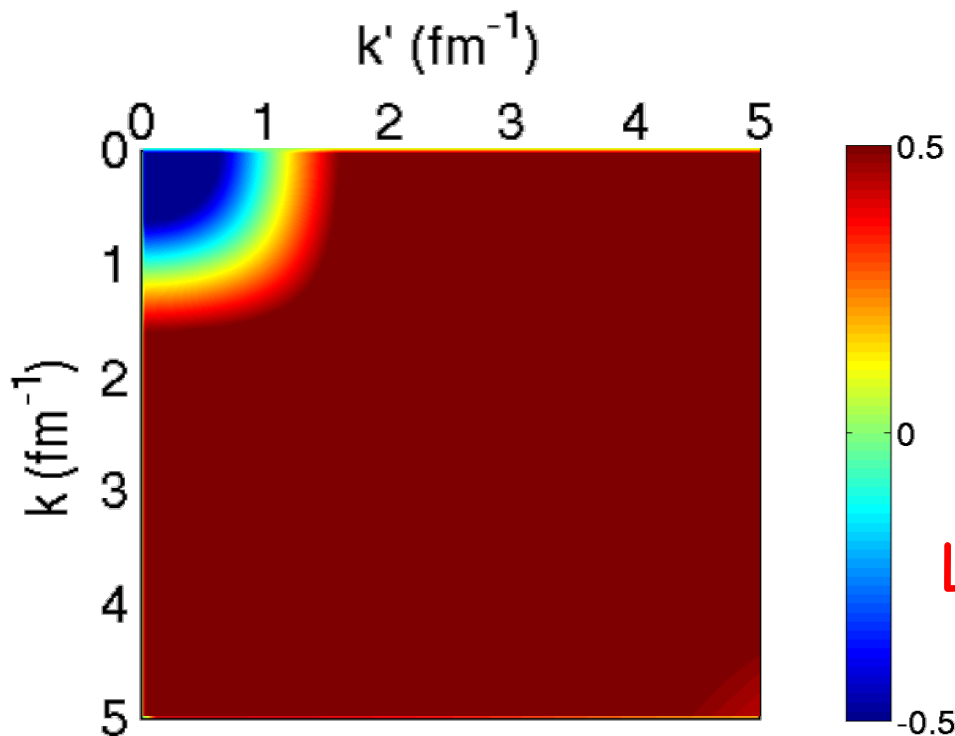
Plane wave

$$\lambda_0 > \lambda_1 > \lambda_2 \dots$$

# Example: Similarity renormalization group (SRG) transformation

$$\tilde{H}_\lambda = U_\lambda H U_\lambda^\dagger$$

$$\frac{d\tilde{H}_\lambda}{d\lambda} = -\frac{4}{\lambda^5} [\eta(\lambda), \tilde{H}_\lambda]$$



$$\langle k | \tilde{H}_\lambda^{(2)} | k' \rangle$$

$$\lambda = 20 \text{ fm}^{-1}$$

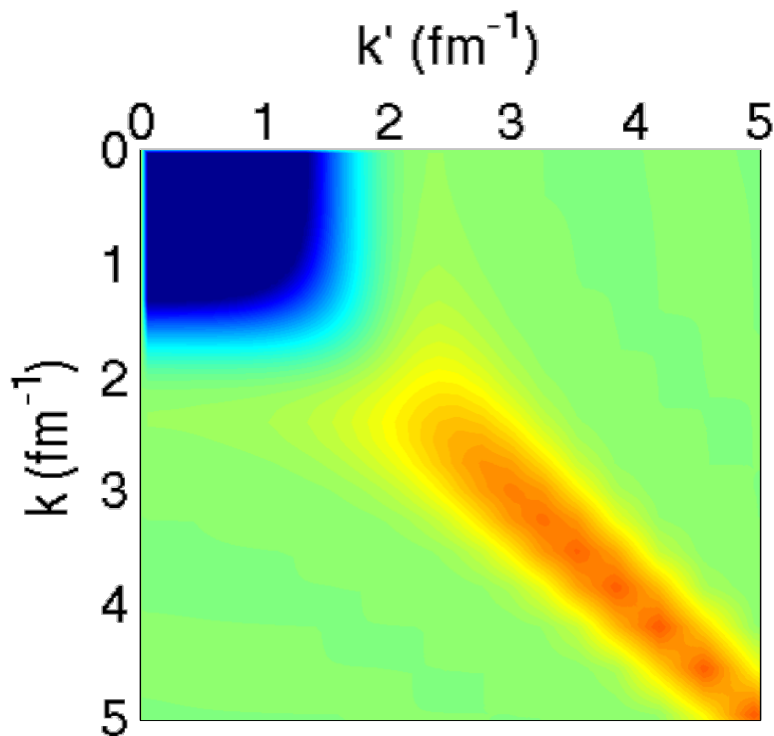
Low and high momentum components coupled

# Example: Similarity renormalization group (SRG) transformation

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$$\tilde{H}_\lambda = U_\lambda H U_\lambda^\dagger$$

$$\frac{d\tilde{H}_\lambda}{d\lambda} = -\frac{4}{\lambda^5} [\eta(\lambda), \tilde{H}_\lambda]$$



$$\langle k | \tilde{H}_\lambda^{(2)} | k' \rangle$$

$$\lambda = 2 \text{ fm}^{-1}$$

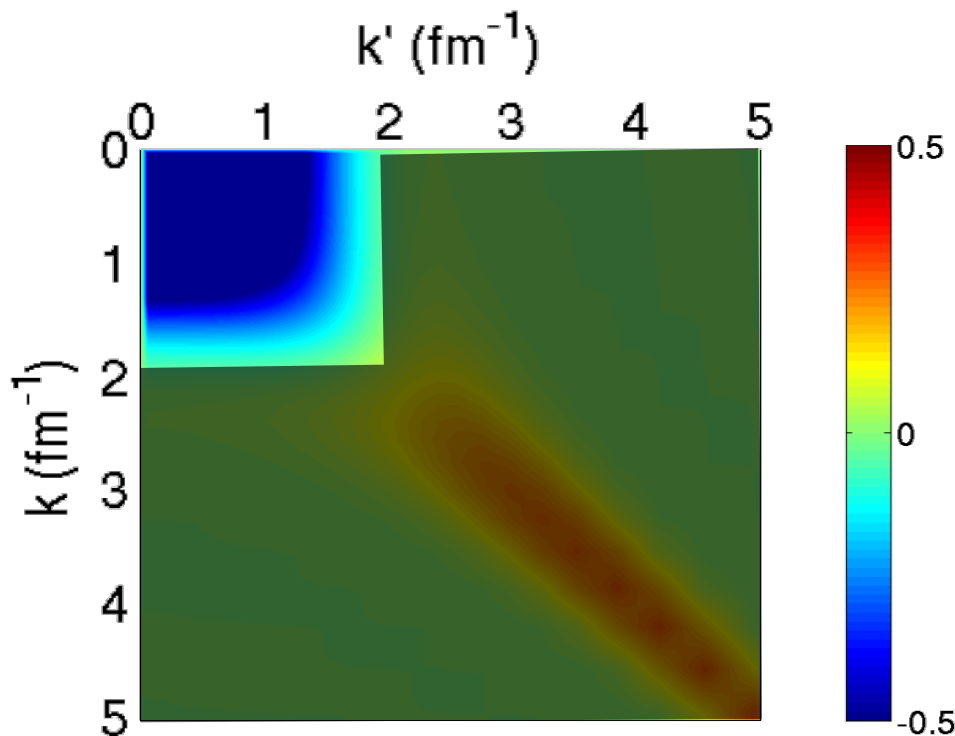
Low and high momentum  
components de-coupled

# Example: Similarity renormalization group (SRG) transformation

---

$$\tilde{H}_\lambda = U_\lambda H U_\lambda^\dagger$$

$$\frac{d\tilde{H}_\lambda}{d\lambda} = -\frac{4}{\lambda^5} [\eta(\lambda), \tilde{H}_\lambda]$$



$$\langle k | \tilde{H}_\lambda^{(2)} | k' \rangle$$

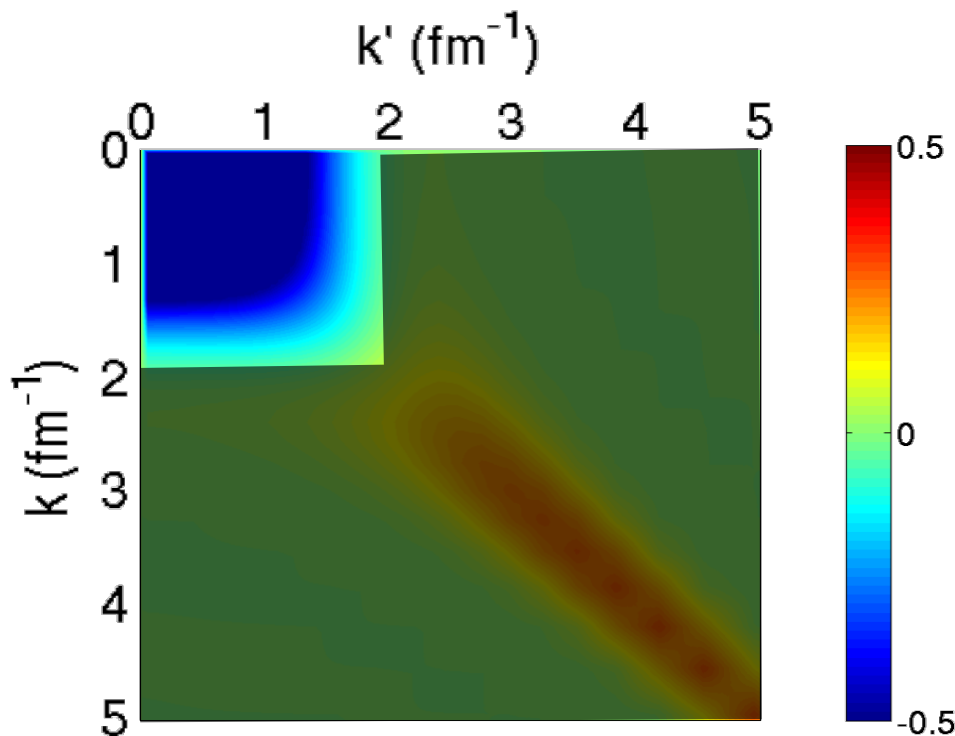
$$\lambda = 2 \text{ fm}^{-1}$$

Can work with smaller  
N values (basis sizes)!

# Example: Similarity renormalization group (SRG) transformation

$$\tilde{H}_\lambda = U_\lambda H U_\lambda^\dagger$$

$$\frac{d\tilde{H}_\lambda}{d\lambda} = -\frac{4}{\lambda^5} [\eta(\lambda), \tilde{H}_\lambda]$$



$$\langle k | \tilde{H}_\lambda^{(2)} | k' \rangle$$

$$\lambda = 2 \text{ fm}^{-1}$$

See: Bogner, Furnstahl, Schwenk,  
Prog. Part. Nucl. Phys. 65 (2010)

# Question

---

- This sounds too good to be true ...
- What's the catch?

# Notes on effective interactions

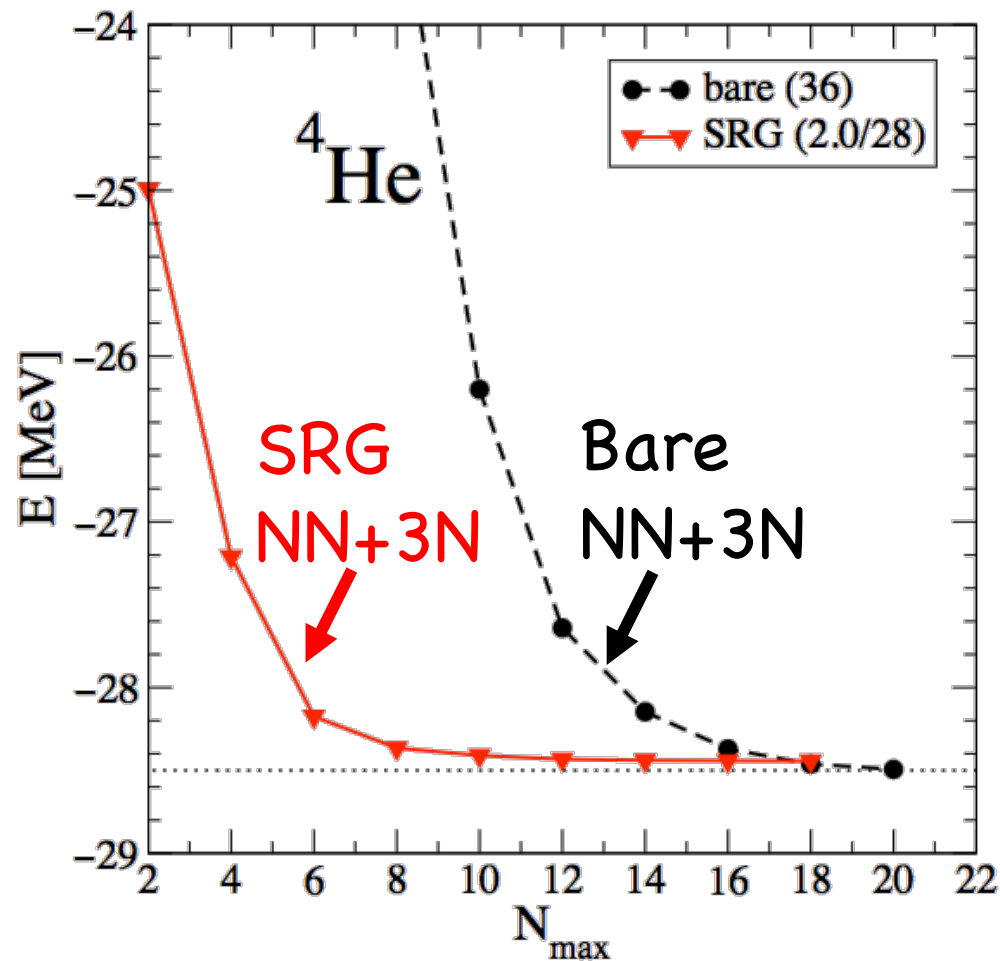
---

- The transformation (e.g., SRG) generates a ‘new’, softer NN interaction
- Unitarily equivalent to the bare NN potential in the two-nucleon sector only!
- Induces 3-body and, in general, up to A-body forces even starting from an NN potential



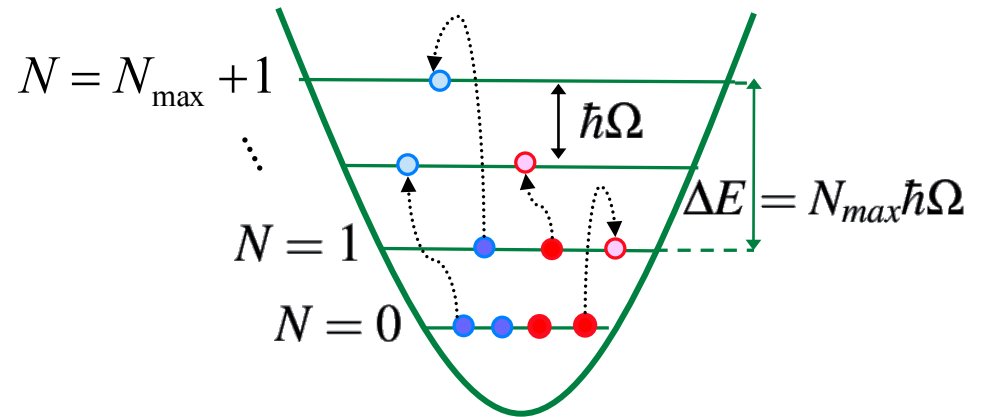
# Example: convergence of ${}^4\text{He}$ ground-state energy with chiral NN+3N forces

Jurgenson et al., PRL 103, 082501



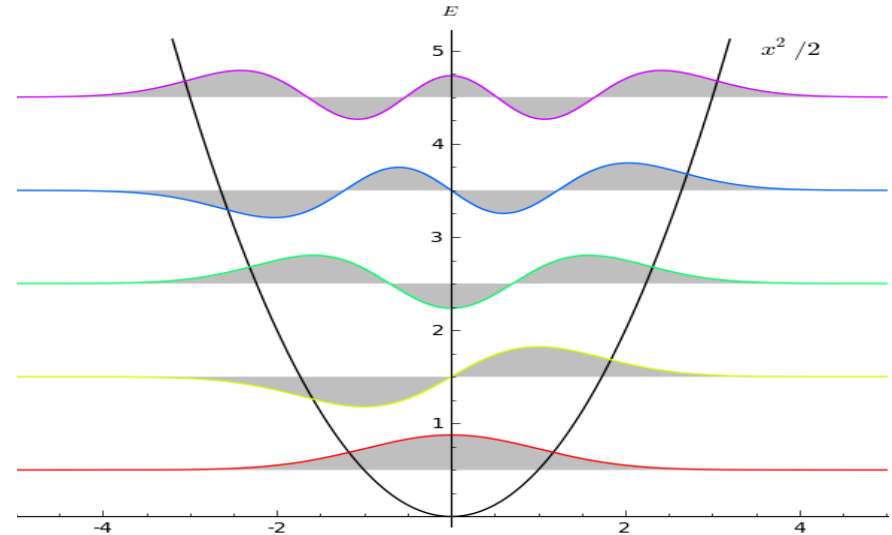
# Ab initio no-core shell model (NCSM)

- Superposition of Harmonic Oscillator (HO) wave functions
- Bare/effective (e.g., SRG) NN+3N forces
- ‘Diagonalizes’ Hamiltonian matrix
- $A \lesssim 16$



# Ab initio no-core shell model (NCSM)

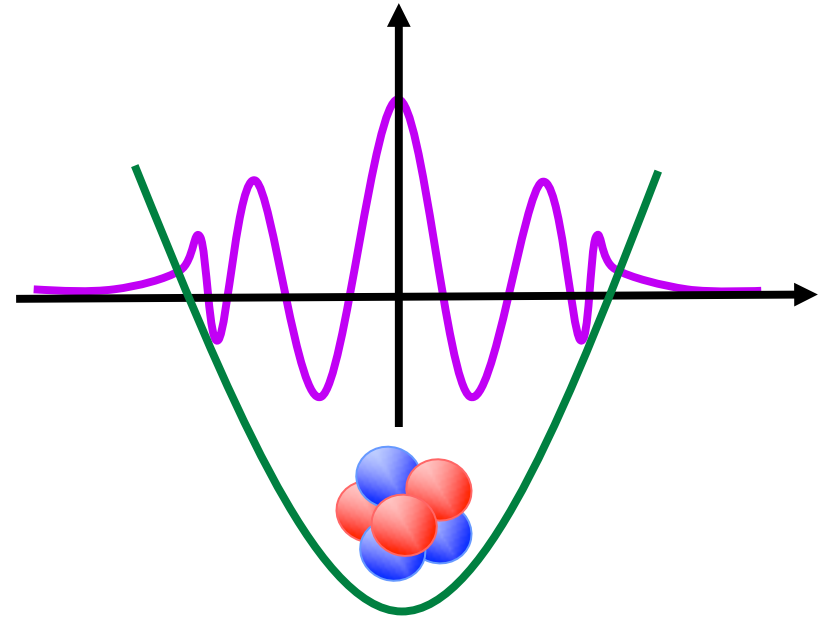
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# Ab initio no-core shell model (NCSM)

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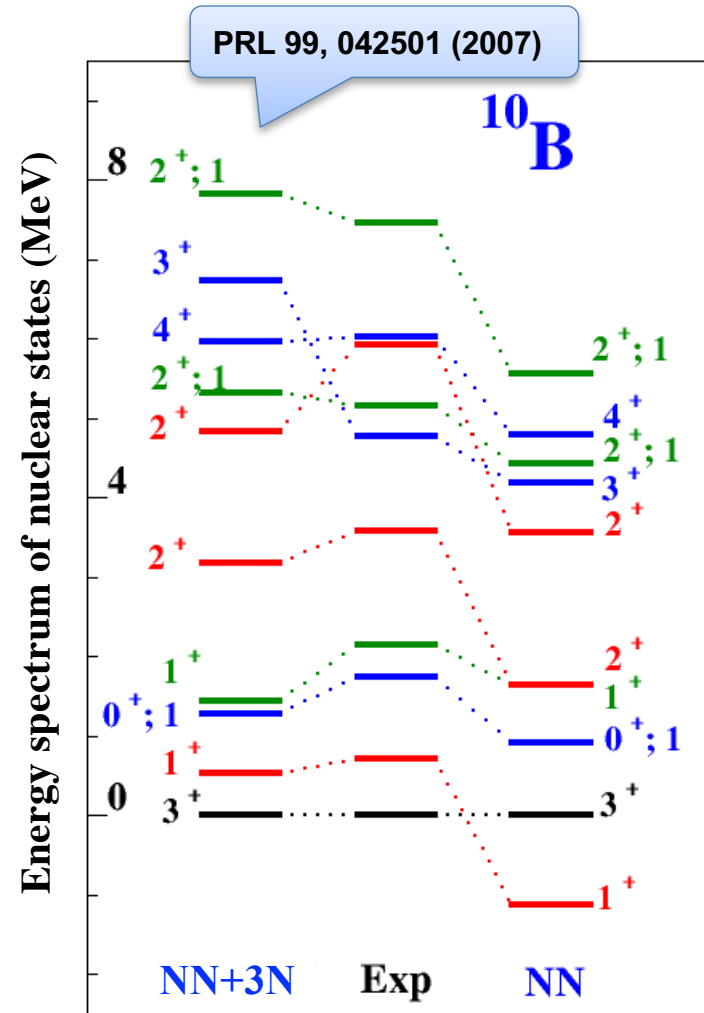


Works well if wave function is localized (well-bound states)

# Ab initio no-core shell model (NCSM)

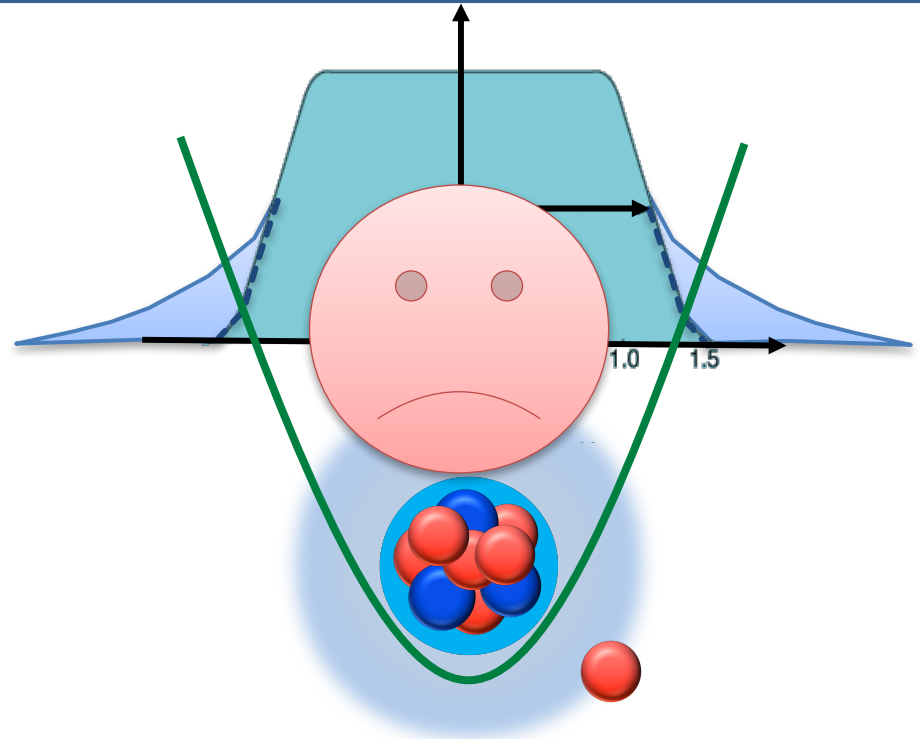
Example: energy spectrum of nuclear states of the  $^{10}\text{B}$  nucleus

Helped to point out the fundamental importance of 3N forces in structure calculations



# Ab initio no-core shell model (NCSM)

- Superposition of Harmonic Oscillator (HO) wave functions
- Bare/effective (e.g., SRG) NN+3N forces
- ‘Diagonalizes’ Hamiltonian matrix
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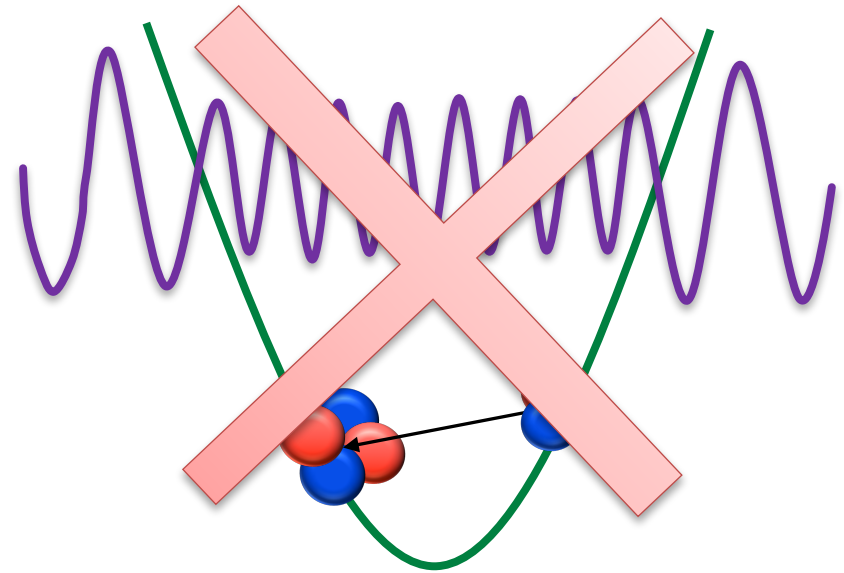


Does not work as well for nuclei with exotic densities (halo nuclei)

# Ab initio no-core shell model (NCSM)

---

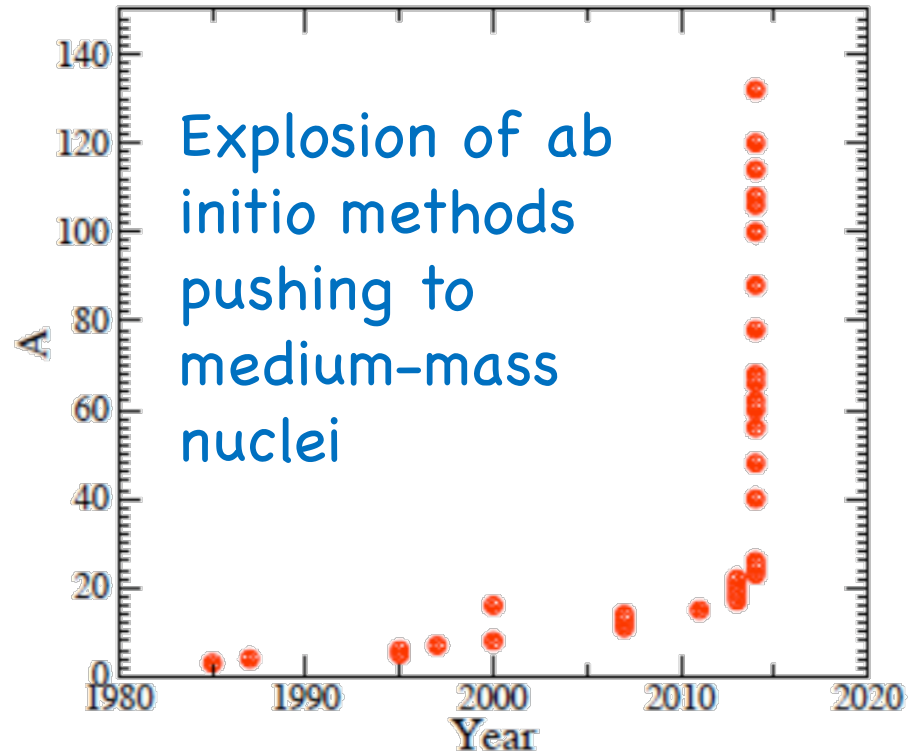
- Superposition of Harmonic Oscillator (HO) wave functions
- Bare/effective (e.g., SRG) NN+3N forces
- ‘Diagonalizes’ Hamiltonian matrix
- $A \lesssim 16$



Definitively not adapted  
to the description of  
scattering wave functions!

# *Ab initio* community extremely successful in describing the static properties of nuclei

- Green's function Monte Carlo
- Nuclear Lattice Effective Field Theory
- Coupled Cluster theory
- In-Medium SRG
- Gorkov-Green function theory
- Many-Body Perturbation Theory
- Ab initio valence-space shell model



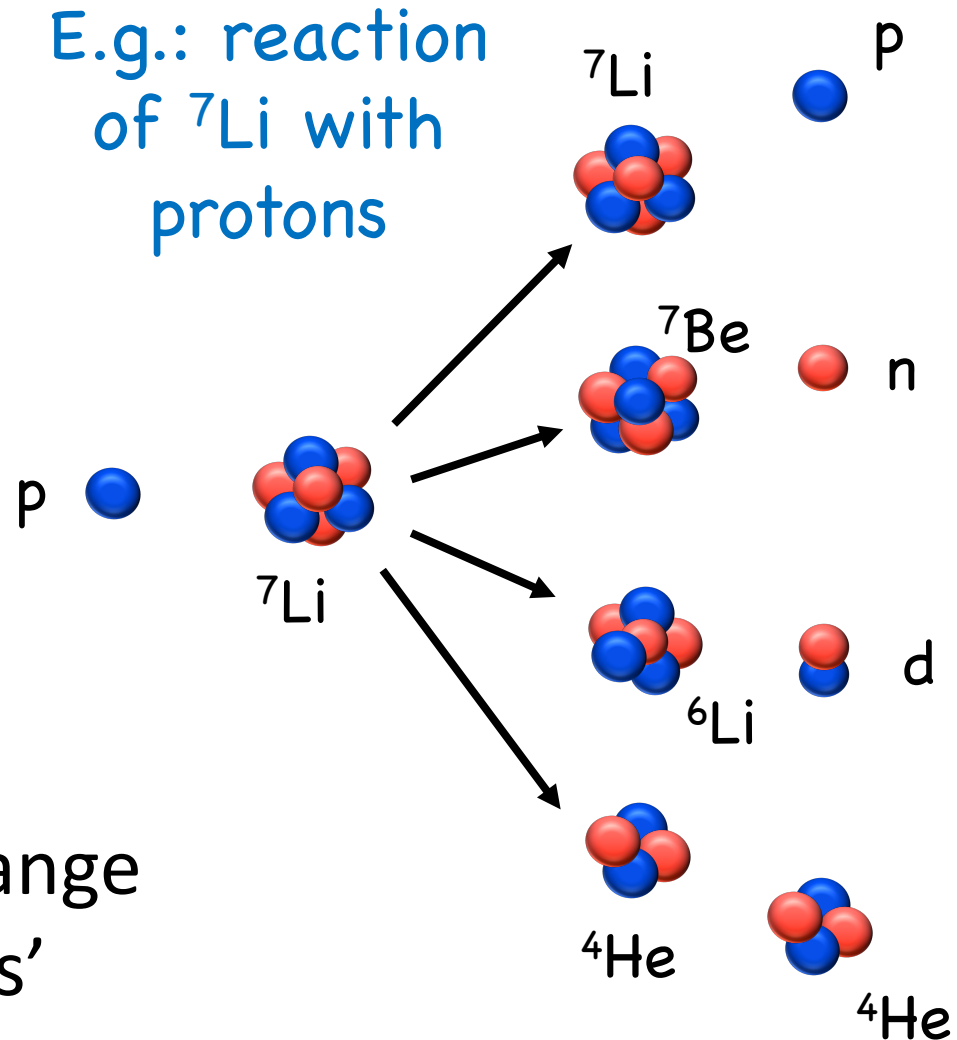
What about the dynamics between nuclei (scattering States with  $E > 0$ )?



How to describe the  
phenomena of low-energy  
nuclear reactions based on  
colliding nuclei made of  
interacting nucleons?

# Problem of nuclear collisions in A-nucleon systems even harder to solve!

- In collisions wave functions extend all over the place
- Simultaneously A-nucleon and projectile-target problem
- Nucleons can re-arrange in different 'channels'



# At low-energy usually only a few reaction channels are open ...

---

$$\Psi = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{cluster} \\ \lambda \end{array} \right\rangle + \sum_{\nu} \int d\vec{r} u_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} \vec{r} \\ \text{cluster} \\ (A-a) \quad (a) \\ \nu \end{array} \right\rangle$$

Unknowns

- We can improve our ansatz for the A-nucleon wave function by further adding ‘microscopic cluster states’ for the relevant reaction channels

# Ab initio no-core shell model with continuum (NCSMC)

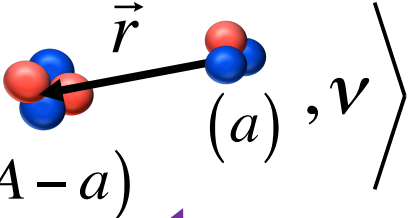
$$\Psi = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{cluster} \end{array}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} u_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} (A-a) \quad (a) \\ \text{cluster} \end{array}, \nu \right\rangle$$

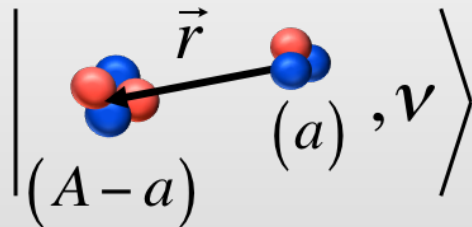

Localized  
A-nucleon  
solutions  
(eigenstates)  
computed with  
the NCSM

$$\left| \begin{array}{c} (A) \\ \text{cluster} \end{array}, \lambda \right\rangle = \sum_k^N b_k^{(\lambda)} \Phi_k(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$$

$$(\mathbf{H}^{(A)} - E_{\lambda}) \left| \begin{array}{c} (A) \\ \text{cluster} \end{array}, \lambda \right\rangle = 0$$

# Ab initio no-core shell model with continuum (NCSMC)

$$\Psi = \sum_{\lambda} c_{\lambda} \left| (A) \text{ [cluster]}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} u_{\nu}(\vec{r}) \hat{A}_{\nu} \left| (A-a) \text{ [cluster]}, (a) \text{ [cluster]}, \nu \right\rangle$$




$$\left| (A-a) \text{ [cluster]}, (a) \text{ [cluster]}, \nu \right\rangle$$

$$= \left| (A-a) \text{ [cluster]}, \nu_1 \right\rangle \left| (a) \text{ [cluster]}, \nu_2 \right\rangle \delta(\vec{r} - \vec{r}_{A-a,a})$$

**Continuous**  
microscopic cluster  
states made of  
projectile-target  
pairs in relative  
motion

# Ab initio no-core shell model with continuum (NCSMC)

---

$$\Psi = \sum_{\lambda} c_{\lambda} \left| (A) \begin{array}{c} \text{projectile} \\ \text{target} \end{array}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} u_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} \text{projectile} \\ \text{target} \end{array}, \nu \right\rangle$$

Sum over relevant reaction channels (mass partitions)

Antisymmetrizes exchanges of nucleons between projectile and target

# Ab initio no-core shell model with continuum (NCSMC)

---

$$\Psi = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{[Cluster of } A \text{ nucleons]} \\ \lambda \end{array} \right\rangle + \sum_{\nu} \int d\vec{r} u_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} \text{[Cluster of } (A-a) \text{ nucleons]} \\ (a) \\ \nu \end{array} \right\rangle$$

Describe efficiently  
the wave function  
when all  $A$  nucleons  
are close together

Describe efficiently  
the wave function  
when the reactants/  
reaction products  
are far apart

# Ab initio no-core shell model with continuum (NCSMC)

---

$$\Psi = \sum_{\lambda} c_{\lambda} \left| (A) \begin{array}{c} \text{cluster} \\ \lambda \end{array} \right\rangle + \sum_{\nu} \int d\vec{r} u_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} \text{cluster} \\ (A-a) \end{array} \begin{array}{c} \vec{r} \\ \text{cluster} \\ (a) \\ \nu \end{array} \right\rangle$$



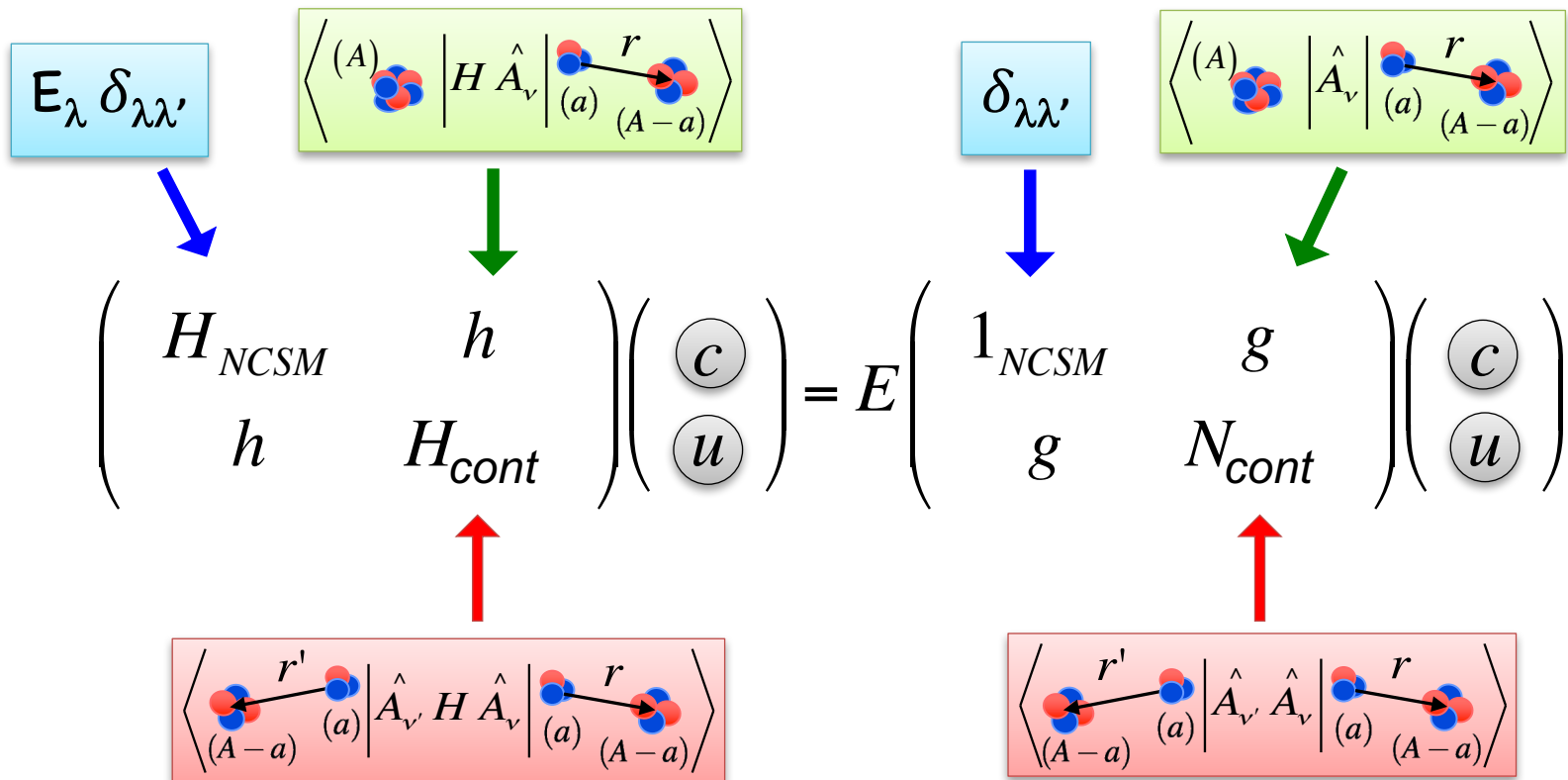
Works well for describing clustering in nuclei (halo nuclei)



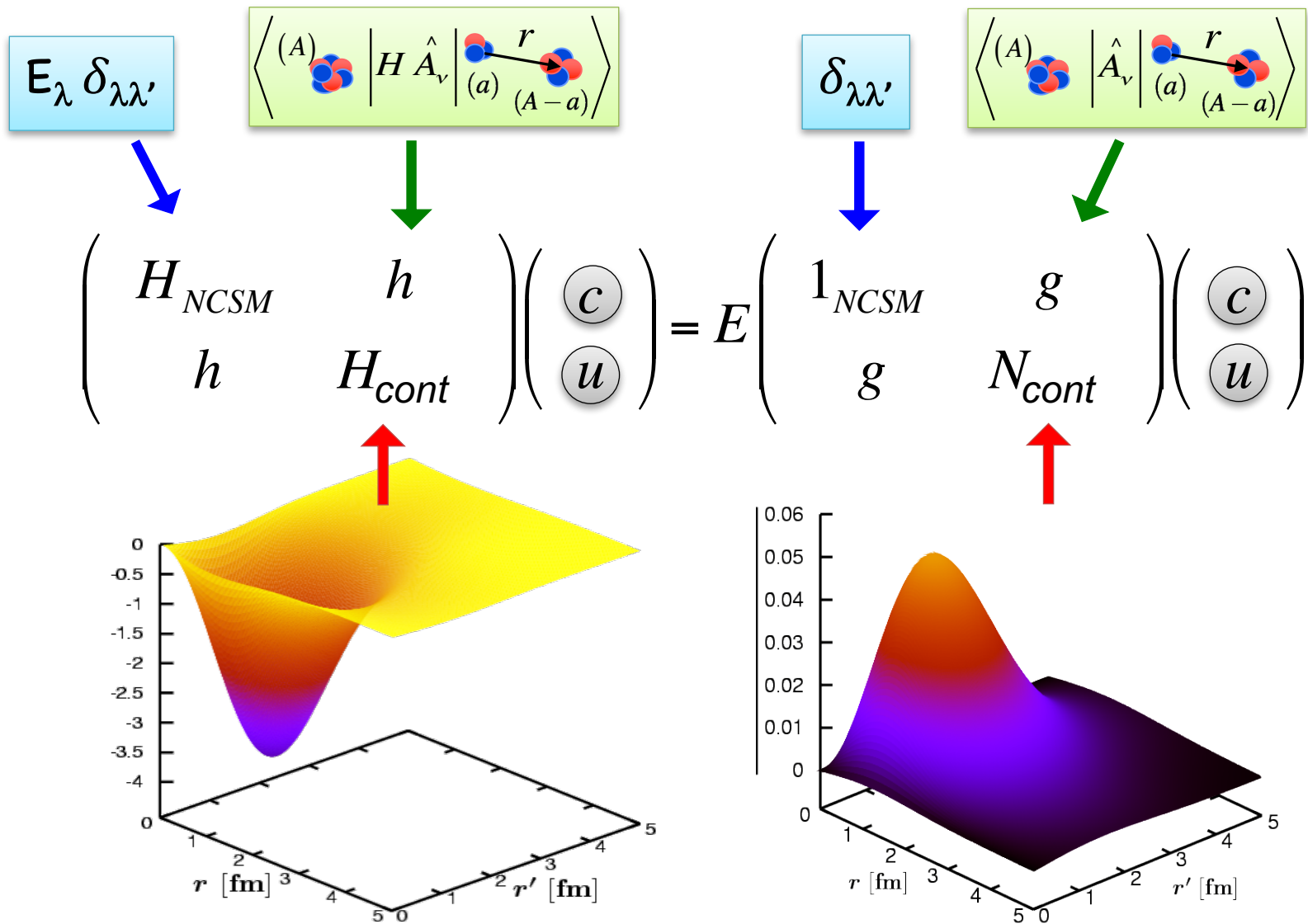
Works well for describing both bound and scattering state



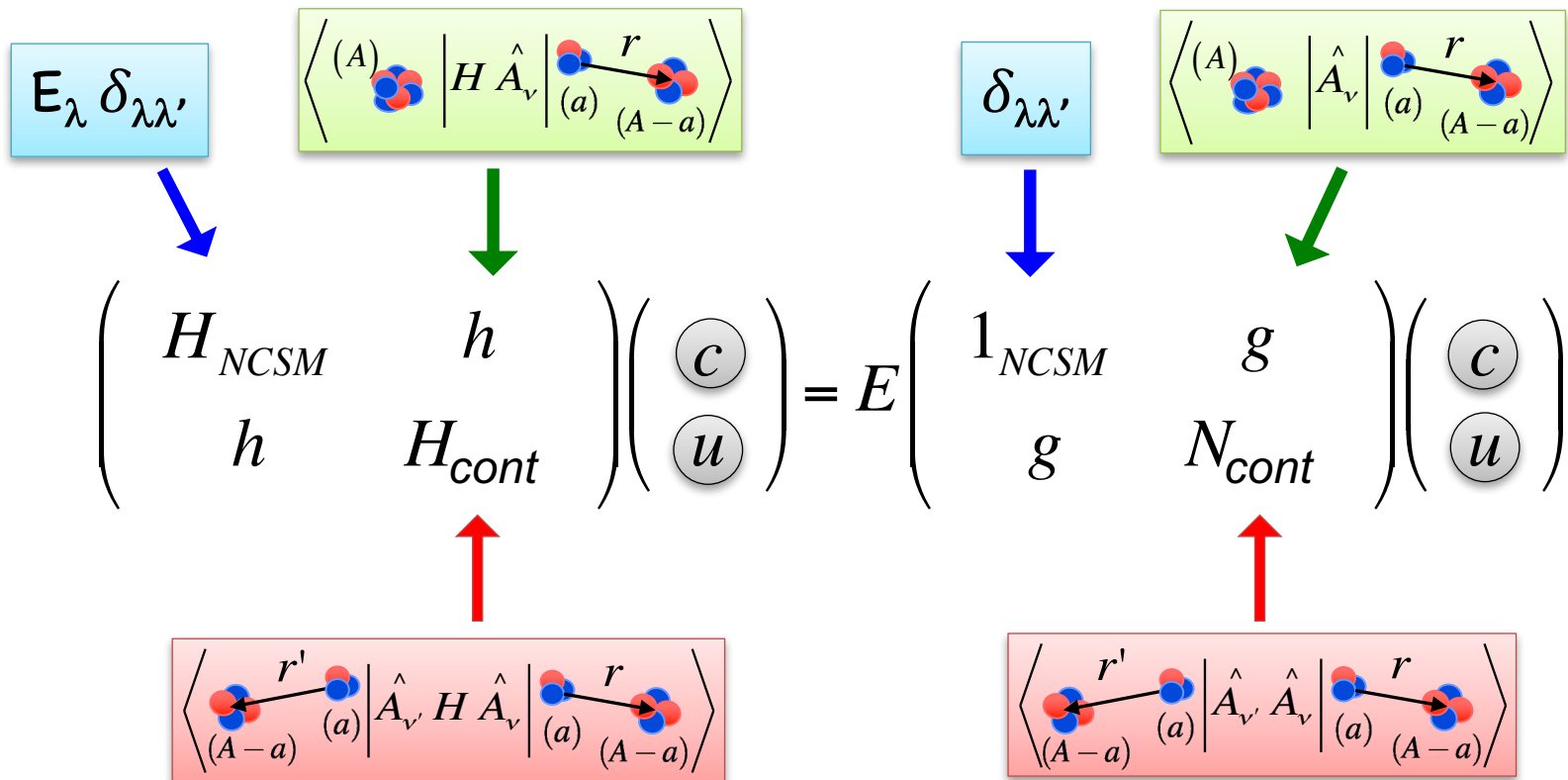
# A-nucleon Schrödinger equation again reduces to an eigenvalue problem



# A-nucleon Schrödinger equation again reduces to an eigenvalue problem



# A-nucleon Schrödinger equation again reduces to an eigenvalue problem

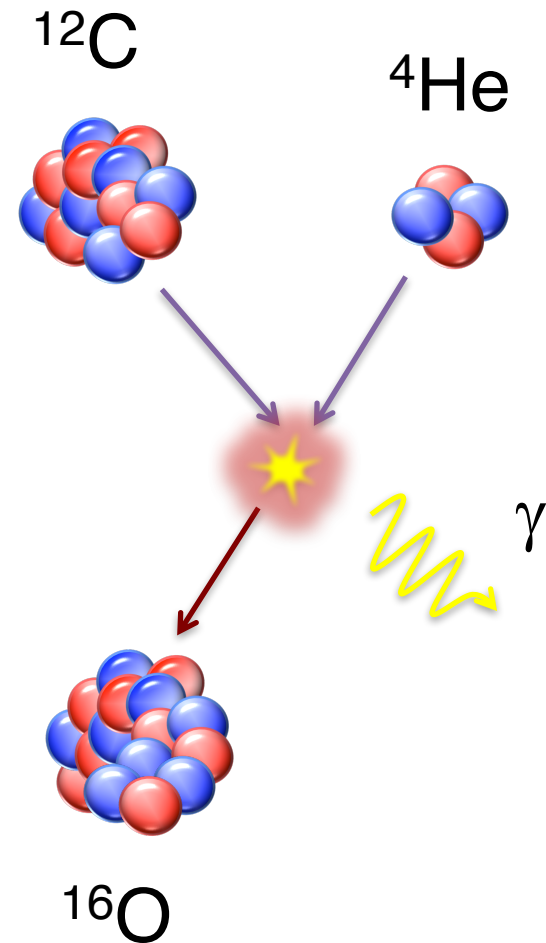


- The spurious center-of mass motion can again be separated exactly (a bit more complicated)

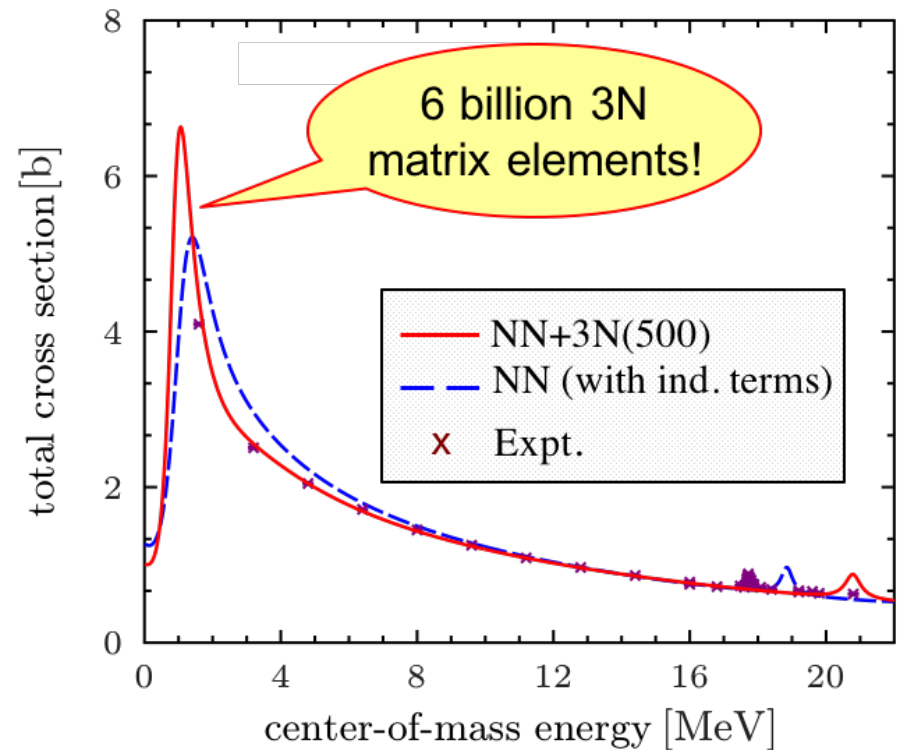
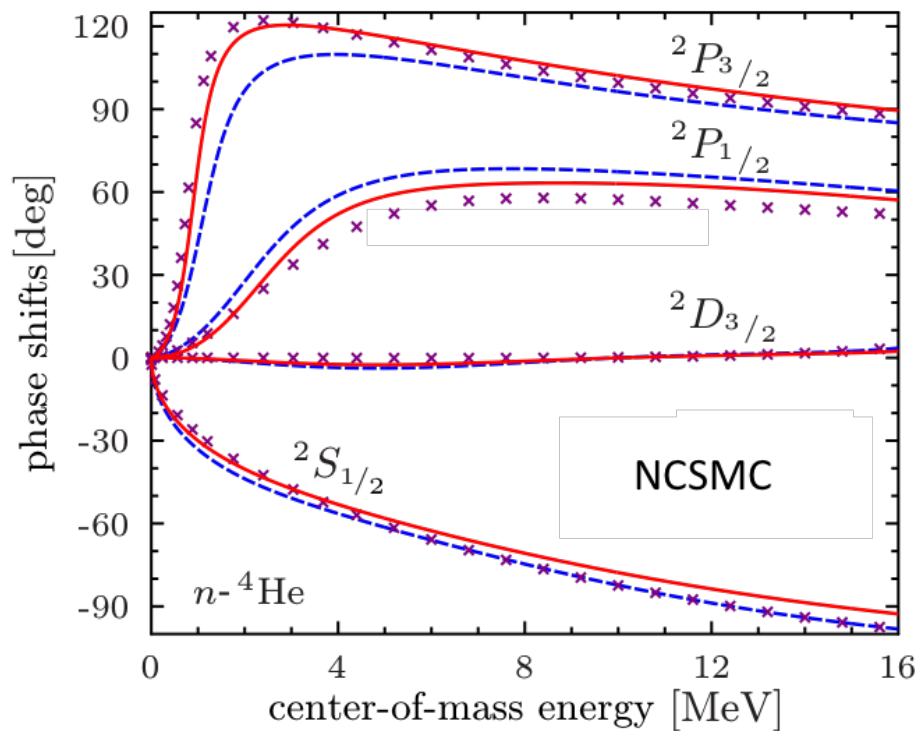
# Question II: Can we predict ...

---

- ... the phenomena of low-energy nuclear reactions based on colliding nuclei made of interacting nucleons?



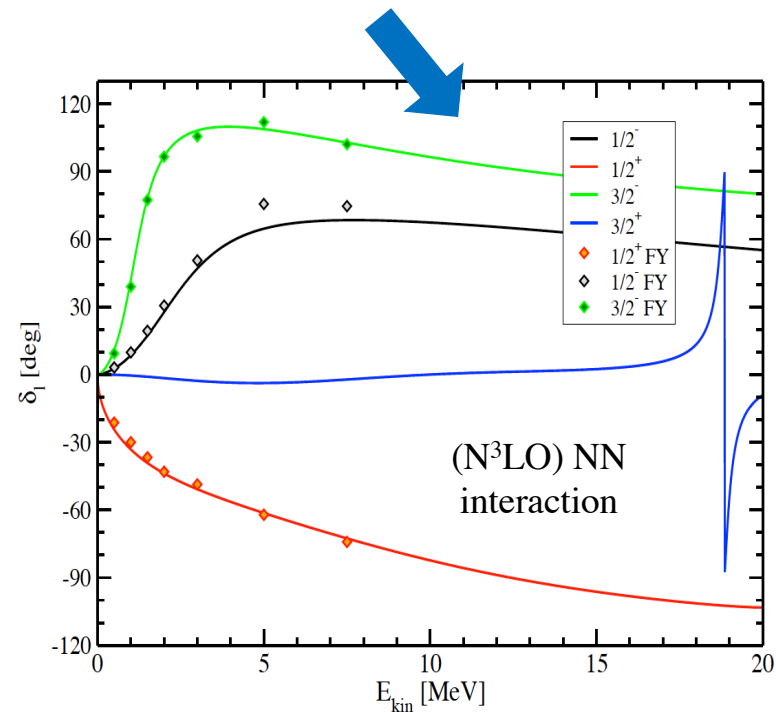
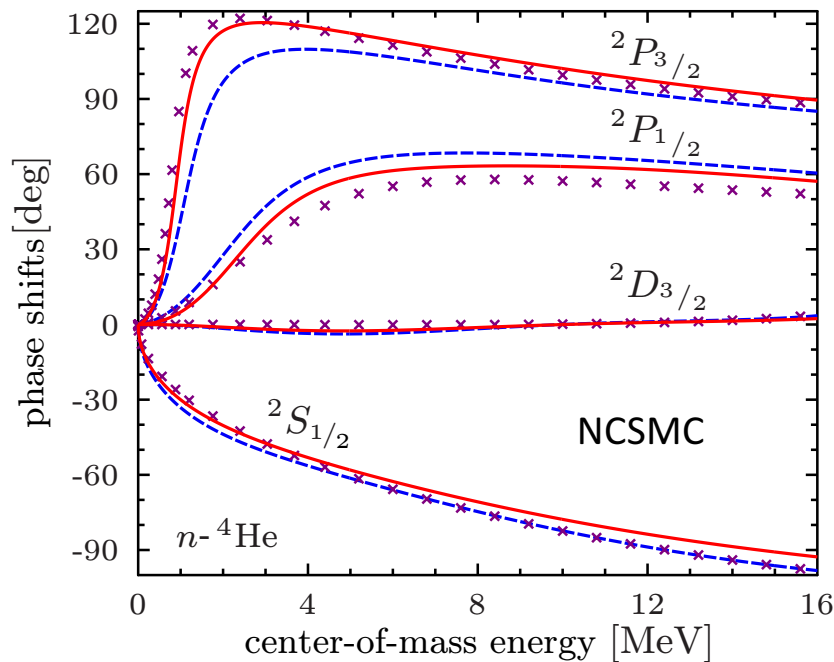
# A good starting point: elastic scattering of neutrons on $^4\text{He}$



G. Hupin, S. Quaglioni, and P. Navratil, JPC Conf. Proc. (2015)

# A good starting point: elastic scattering of neutrons on $^4\text{He}$

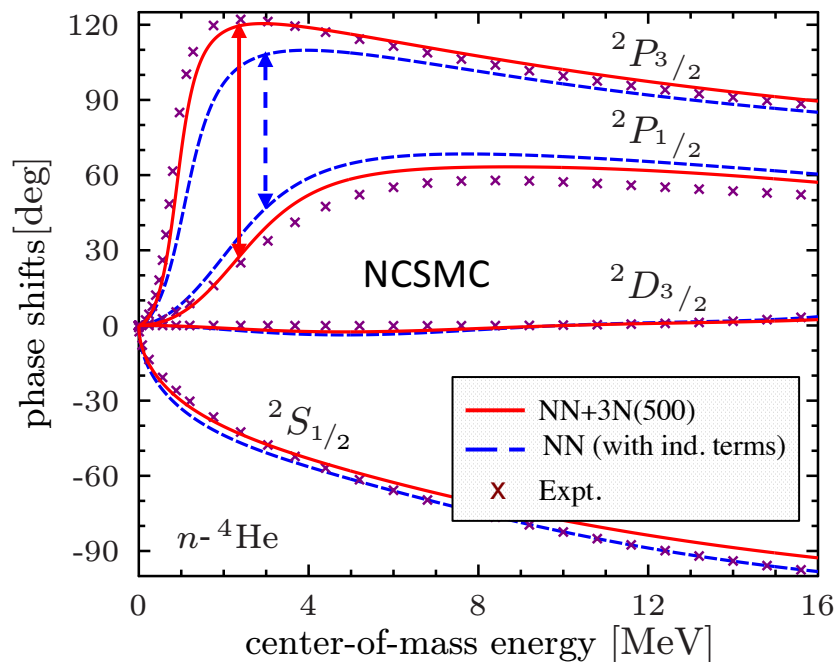
- New 5-body Faddeev-Yacubovsky (FY, symbols) calculations from R. Lazauskas (ongoing work), in very good agreement with the NCSMC results (solid lines)



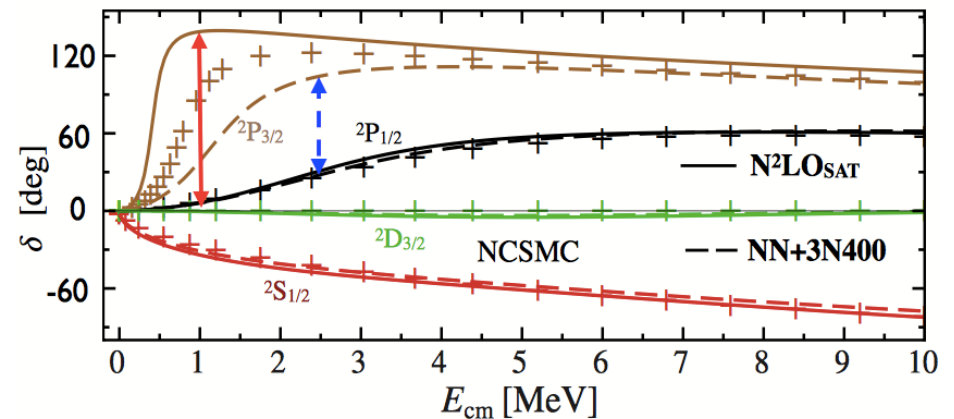
R. Lazauskas, INT Program 17-1a

# A good starting point: elastic scattering of neutrons on $^4\text{He}$

G. Hupin, S. Quaglioni, and P. Navratil,  
JPC Conf. Proc. (2015)



- The 3N force enhances the splitting between the 1/2- and 3/2- phase shifts

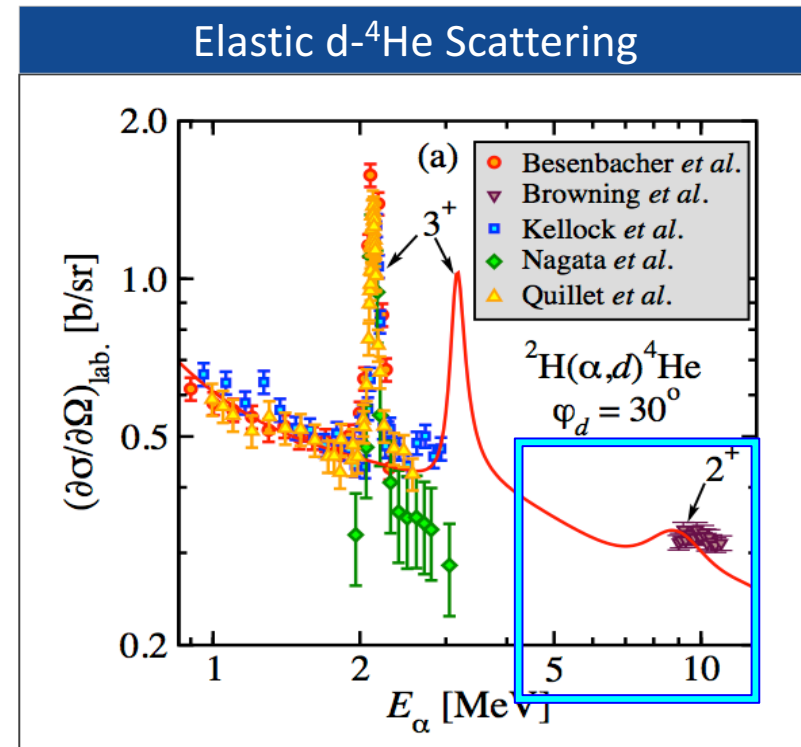
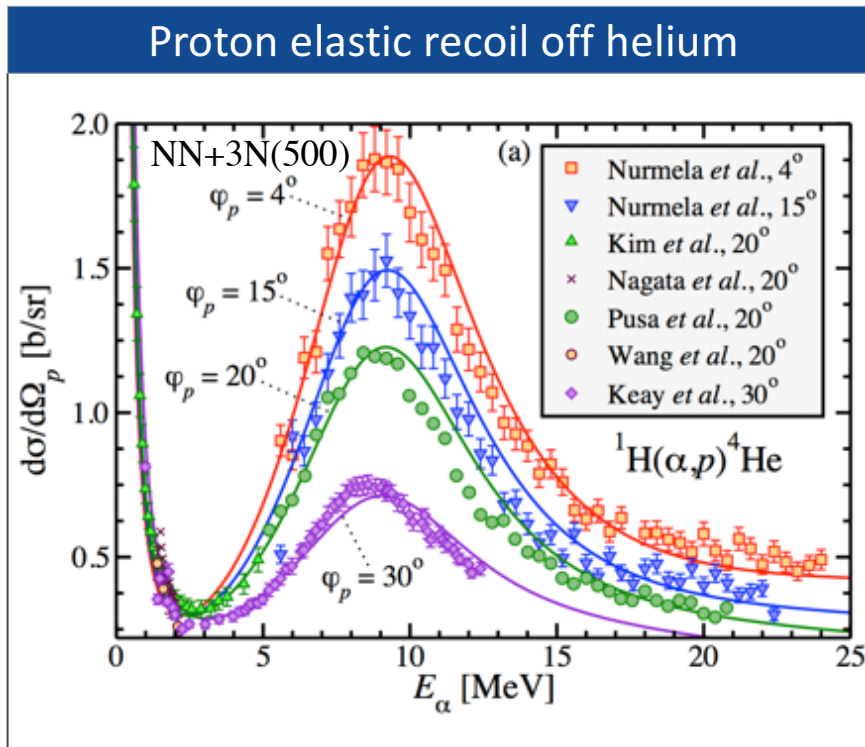


$n-^4\text{He}$  scattering represents a stringent test for nuclear interaction models, and can be used in the future to better constrain chiral NN+3N forces

# We can now predict nucleon and deuterium scattering on $^4\text{He}$ based on chiral NN+3N forces

G. Hupin, S.Q., and P. Navratil,  
Phys. Rev. C **90**, 061601(R) (2014)

G. Hupin, S.Q., and P. Navratil,  
Phys. Rev. Lett. **114**, 212502 (2015)



Chiral NN+3N forces works well, but not everywhere!



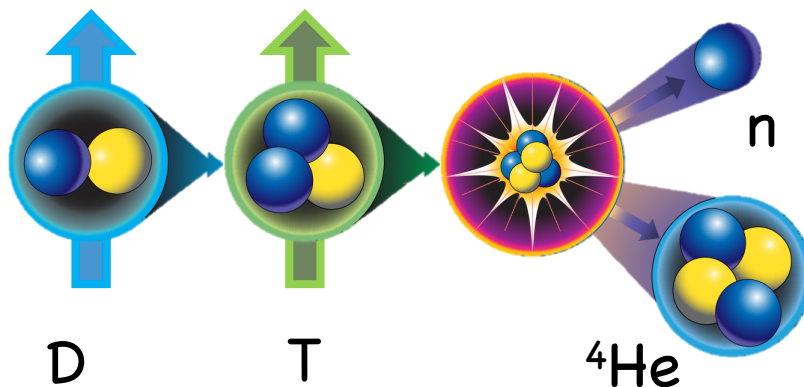
# With the same NN+3N forces, we can also make predictions for more complex transfer reactions

- What is the effect of spin polarization on the DT reaction rate?

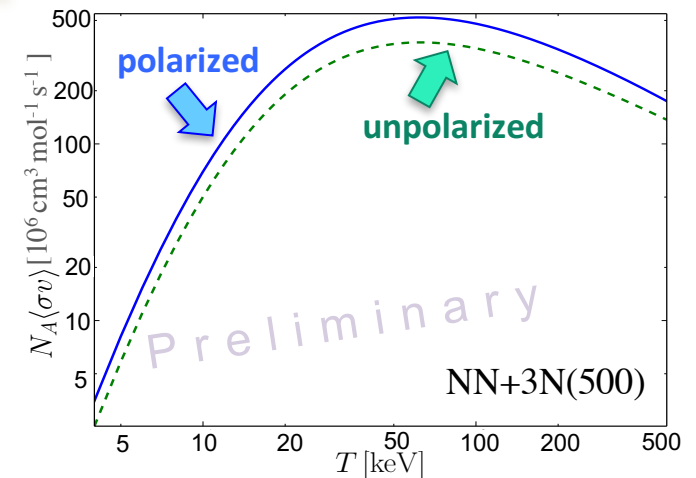
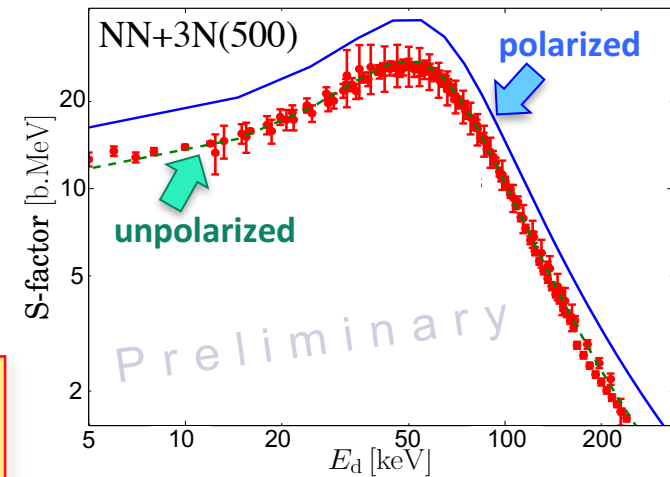


G. Hupin

$$N_A \langle \sigma v \rangle = \sqrt{\frac{8}{\pi \mu}} \frac{N_A}{(k_B T)^{3/2}} \int_0^\infty dE S(E) \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2mE}} - \frac{E}{k_B T}\right)$$

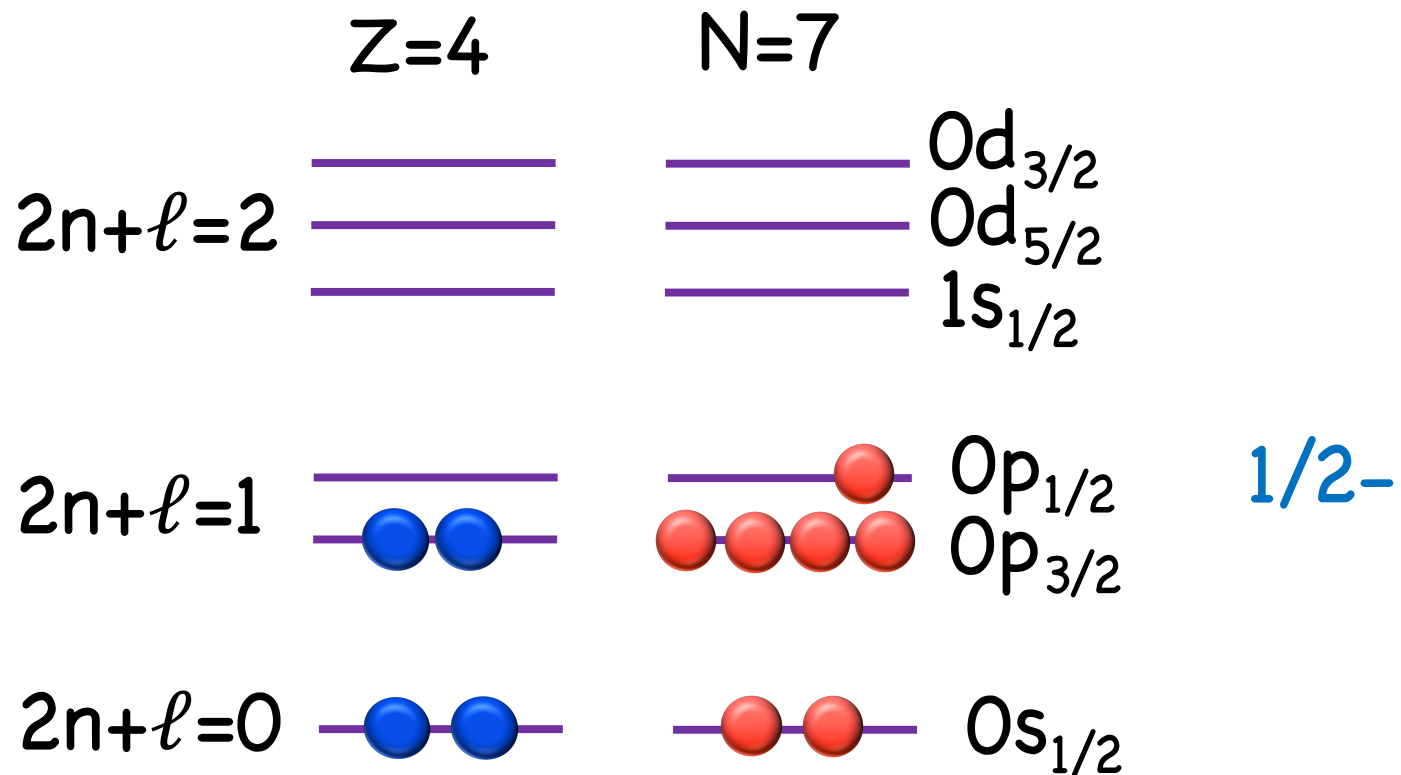


G. Hupin, S. Quaglioni, and P. Navrátil, in progress

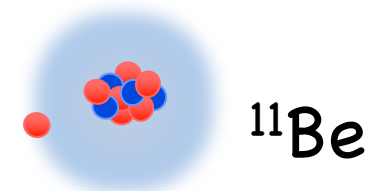
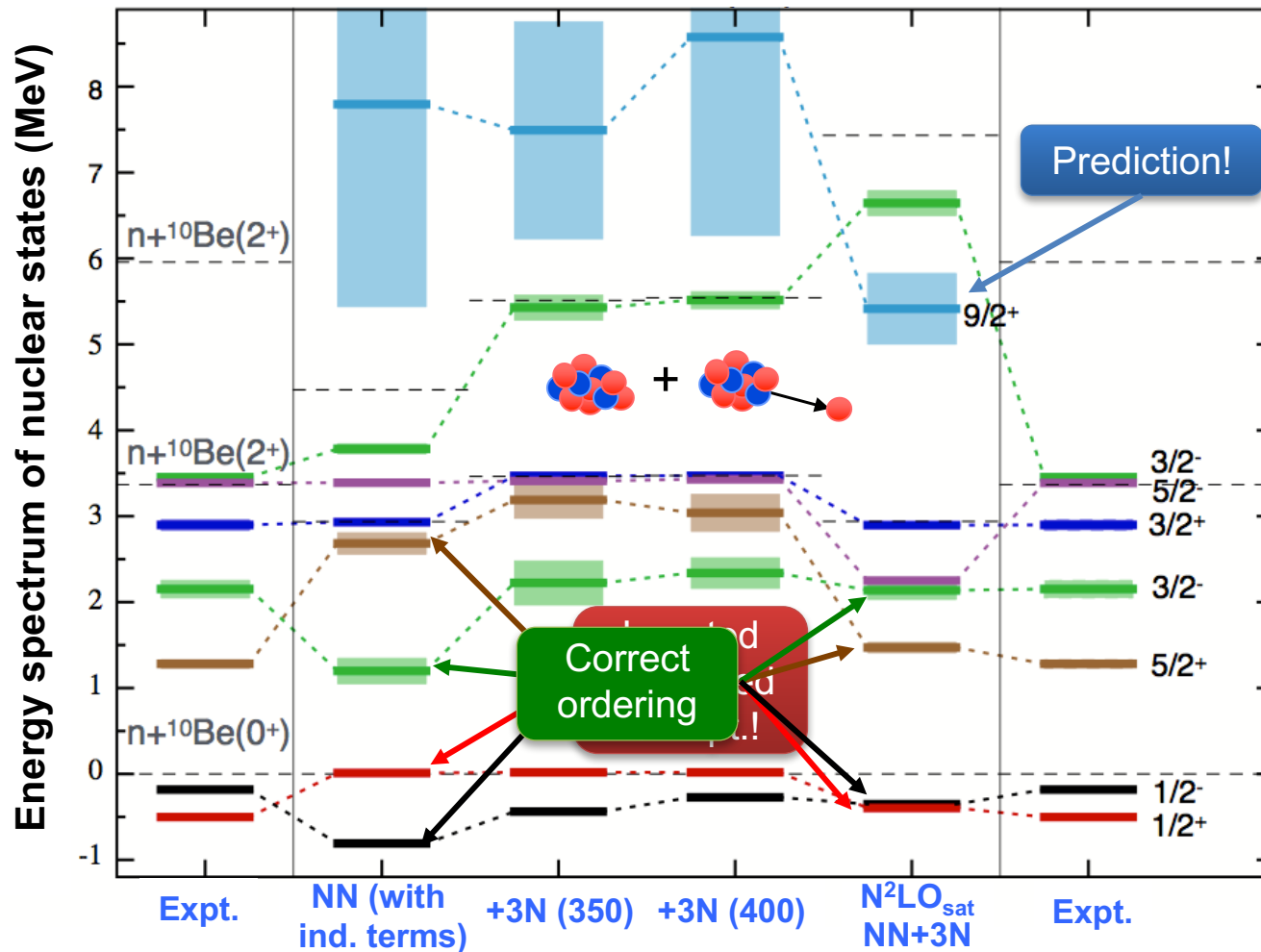


# Problem

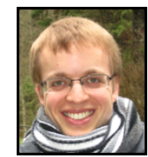
- What is the spin-parity of the ground state of the  $^{11}\text{B}$  nucleus?



# Can ab initio theory explain the phenomenon of parity inversion in $^{11}\text{Be}$ ?



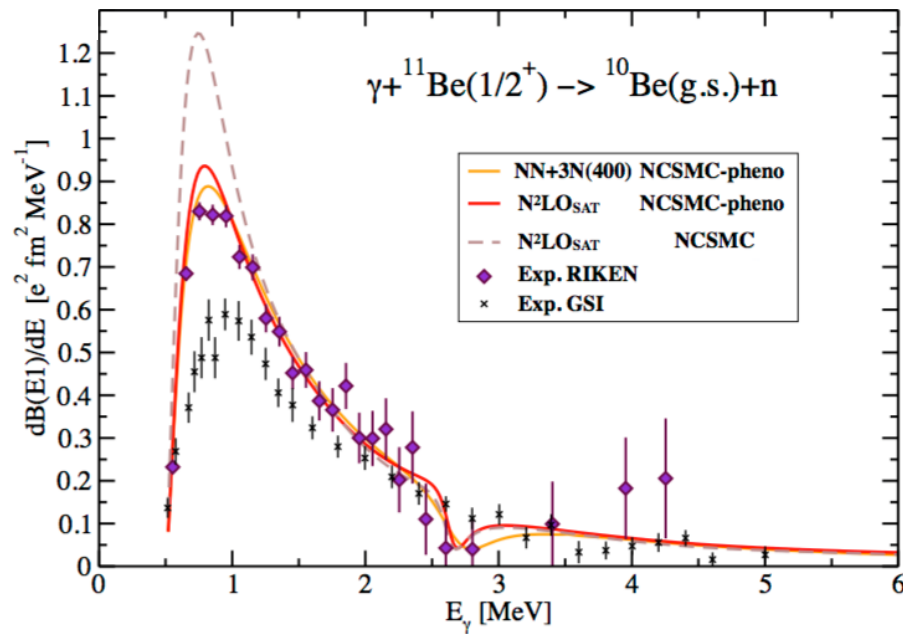
A. Calci



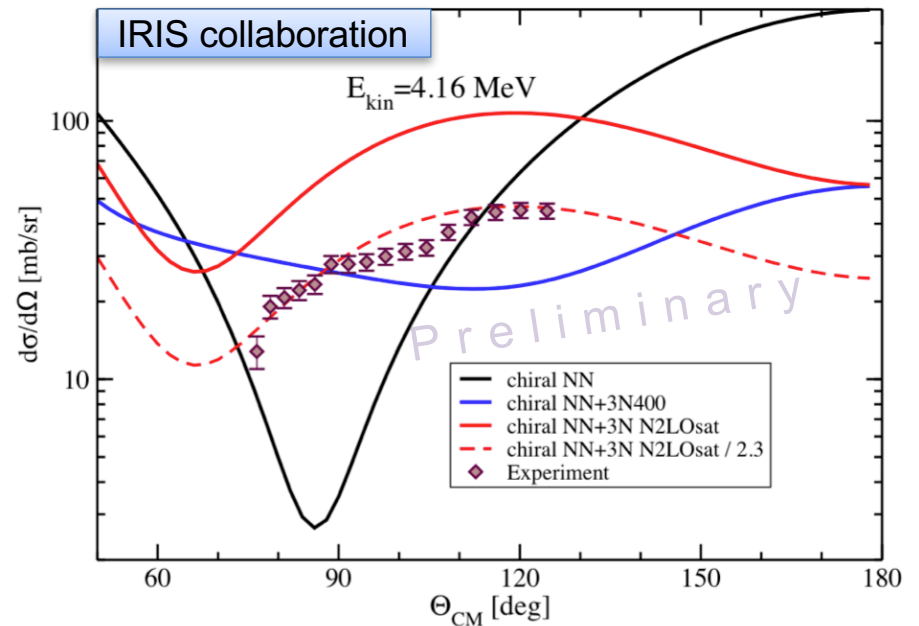
J. Dohet-Eraly

A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S.Q., and G. Hupin, Phys. Rev. Lett. 117, 242501 (2016)

# Scattering and reactions in $A = 11$

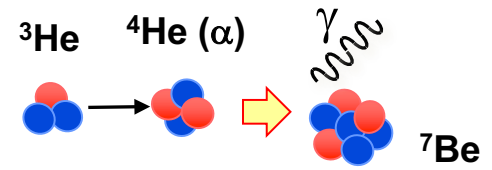


A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S.Q., and G. Hupin, Phys. Rev. Lett. 117, 242501 (2016)



A. Kumar, R. Kanungo, A. Calci, P. Navratil et al., to appear shortly in Phys. Rev. Lett.

# Now gradually building up capability to describe solar pp-chain reactions

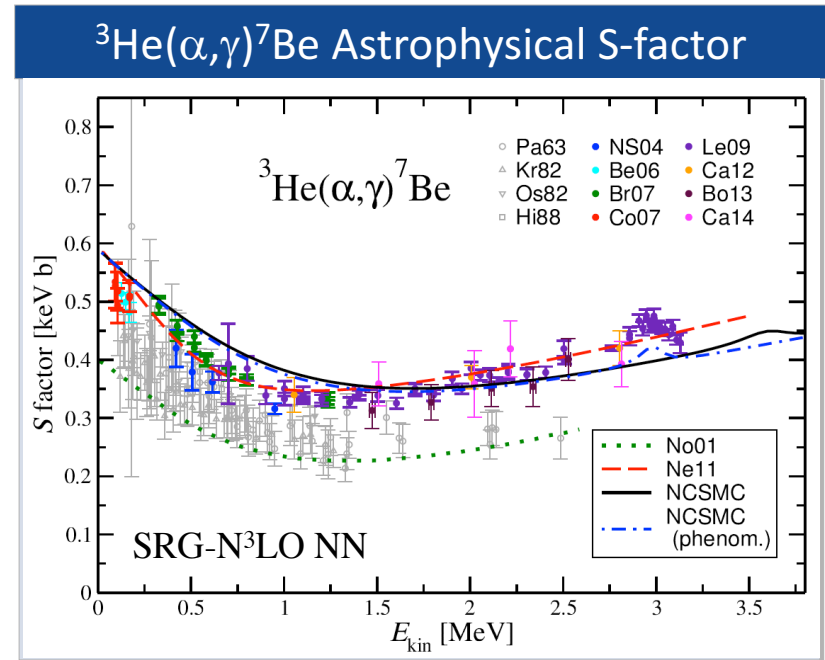
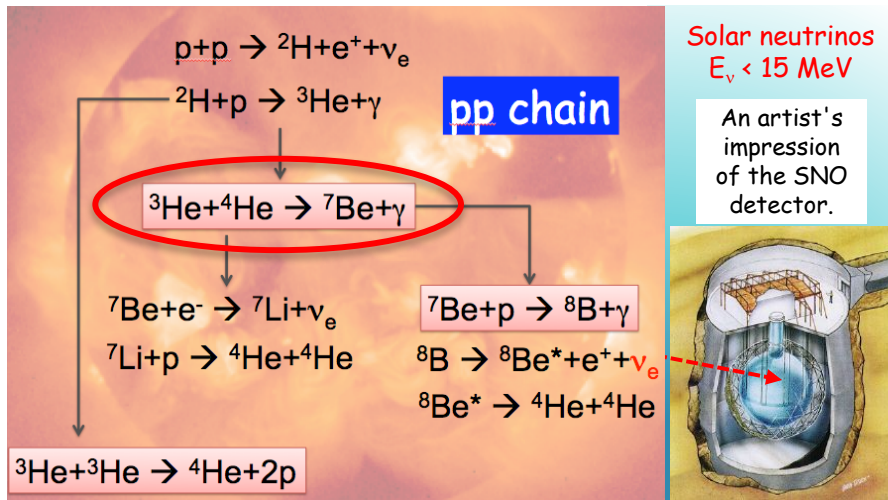


The  ${}^3\text{He}(\alpha, \gamma){}^7\text{Be}$  fusion essential to simulate the flux of solar neutrinos



J. Dohet-Eraly

J. Dohet-Eraly, P. Navrátil, S.Q., W. Horiuchi, and F. Raimondi, *Physics Letters B* **757**, 430 (2016)



Quantitative comparison still requires inclusion of 3N forces

# What about helium burning reactions?

## Nuclear Lattice EFT with the Adiabatic Projection Method

- Use projection Monte Carlo to 'dress' clusters

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

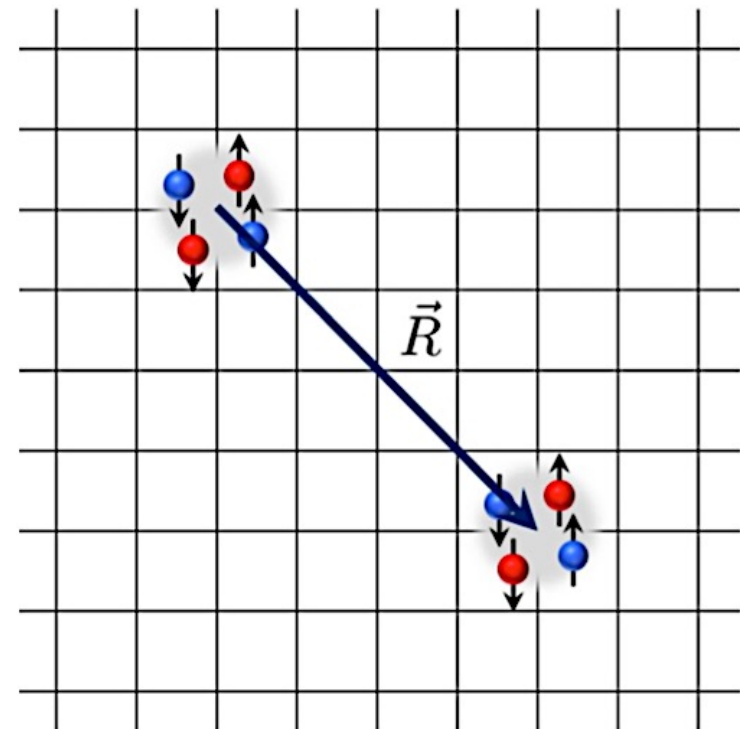
- Evaluate adiabatic inter-cluster Hamiltonian, norm matrix elements

$$[H_\tau]_{\vec{R},\vec{R}'} = \tau \langle \vec{R} | H | \vec{R}' \rangle_\tau$$

$$[N_\tau]_{\vec{R},\vec{R}'} = \tau \langle \vec{R} | \vec{R}' \rangle_\tau$$

- Solve for relative scattering wave function

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r} + \vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$

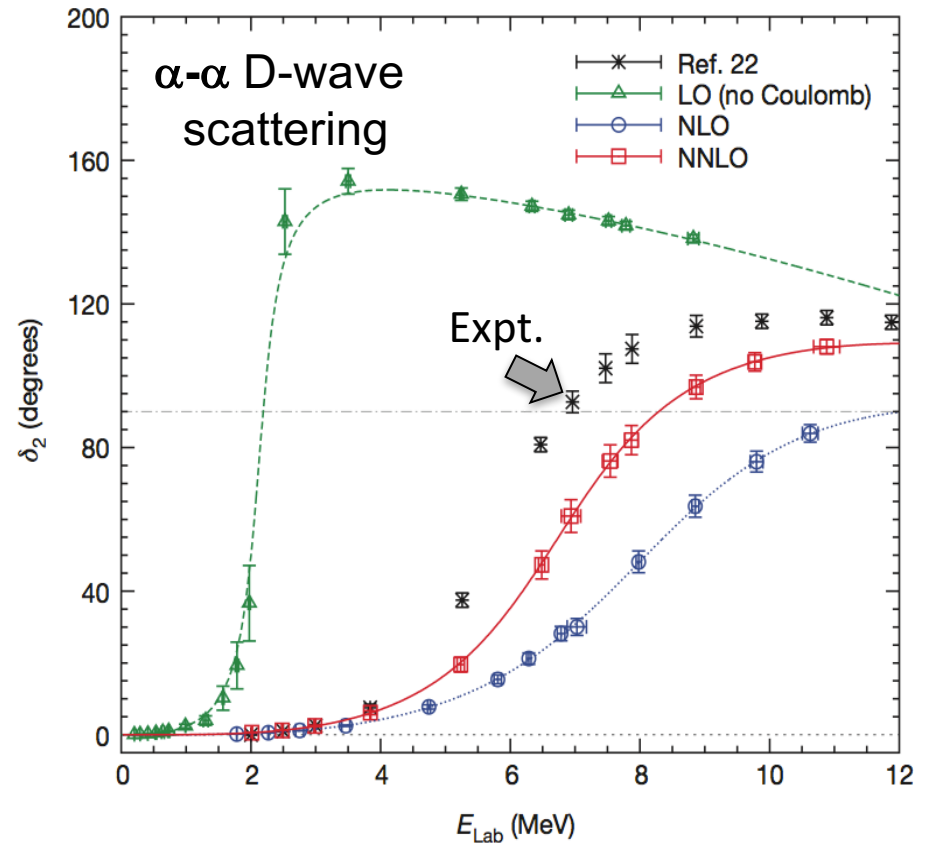


Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)

# Towards ab initio calculations of helium burning

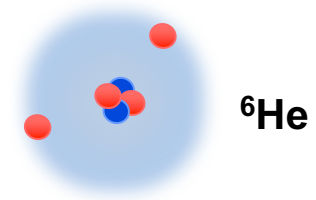
## Nuclear Lattice EFT with the Adiabatic Projection Method

- Promising results for  $\alpha$ - $\alpha$  scattering
- Quantitative predictions still require calculation at N<sup>3</sup>LO
- Computational scaling  $\sim A^2$
- $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$  becoming possible!
- Extensions to enable treatment of three-cluster dynamics required before the method can be applied to the  $^4\text{He}(\alpha\alpha, \gamma)^{12}\text{C}$  process

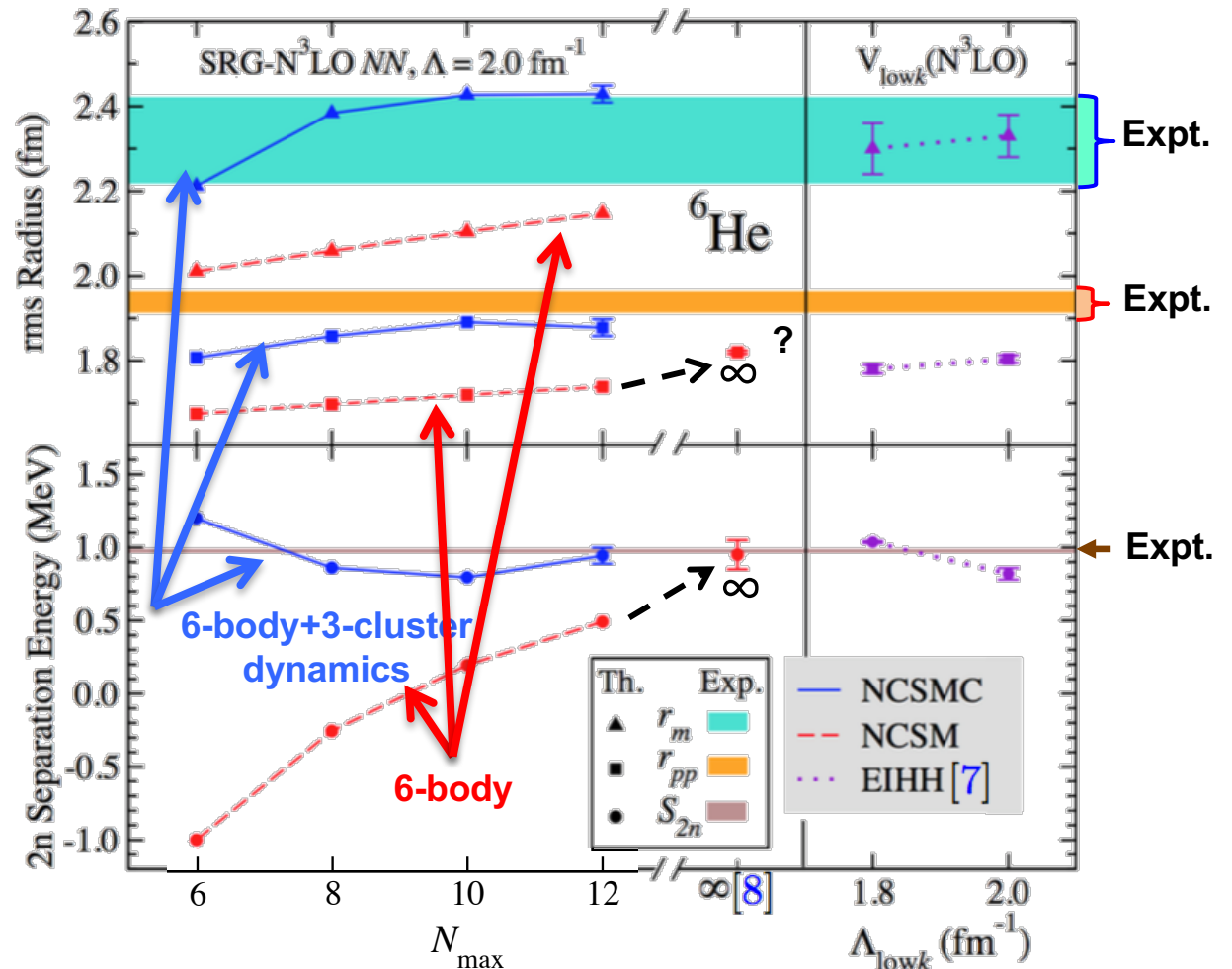
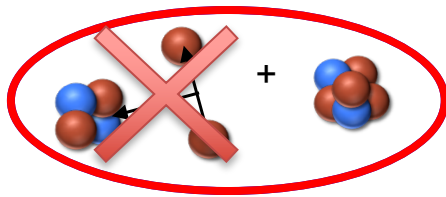


Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)

# How many-body correlations and $\alpha$ -clustering shape ${}^6\text{He}$



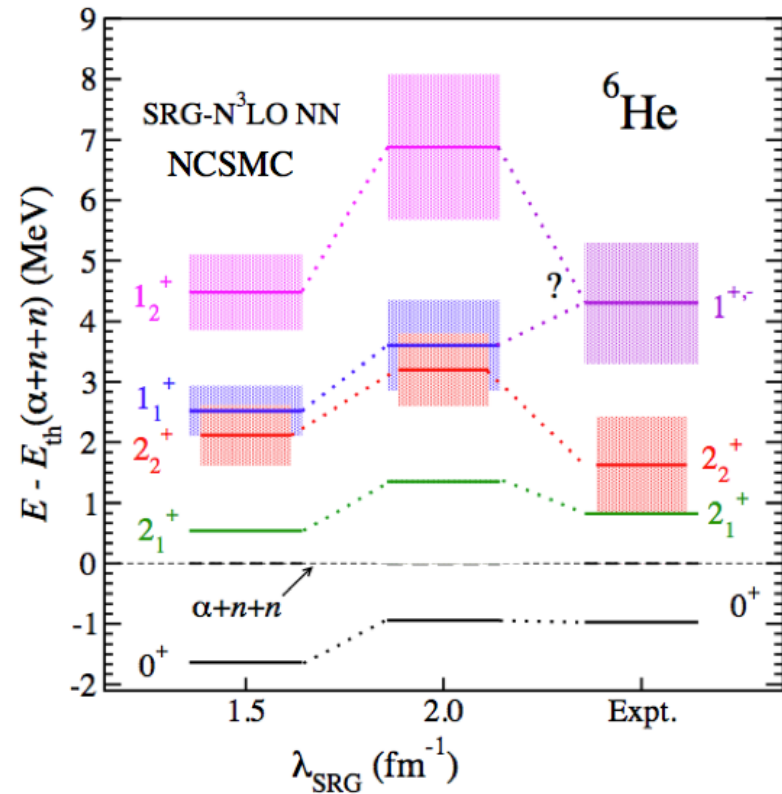
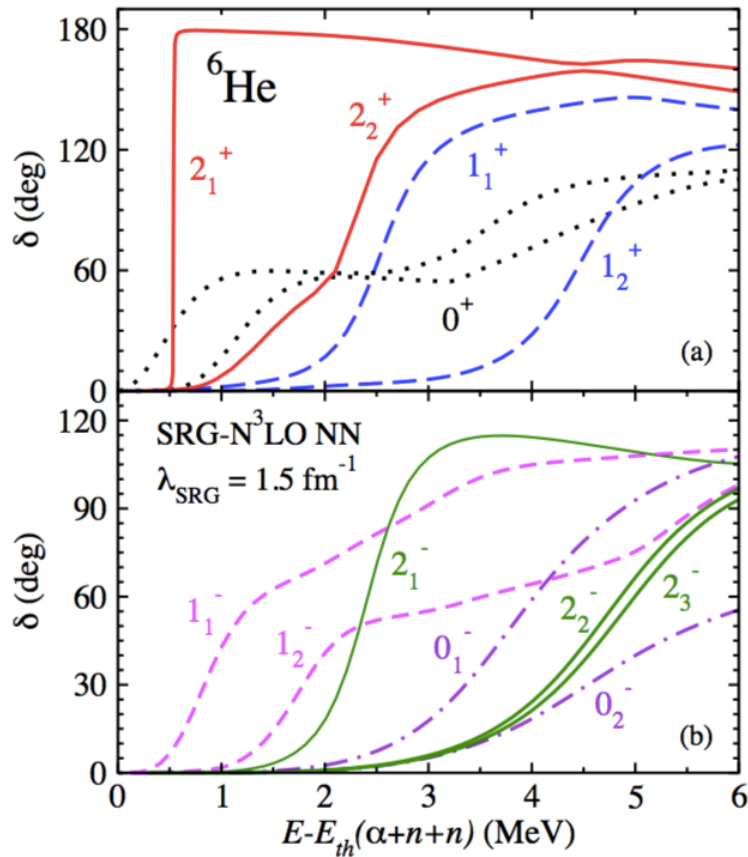
- Stringent tests for *ab initio* theory
- 3-cluster NCSMC



C. Romero-Redondo, S.Q., P.Navratil, and G. Hupin,  
Phys. Rev. Lett. 117, 222501 (2016)



# Results for ${}^6\text{He}$ low-energy continuum



For now, qualitative agreement with experiment. Inclusion of 3N forces (currently underway) remains crucial to arrive at accurate description of the spectrum as a whole.

# Conclusions and Prospects

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- In recent years ab initio theory has made great strides in its description of light-nuclei scattering and reactions as well as of the structure of loosely bound and unbound exotic nuclei
- We are on the verge of predicting Solar fusion and Helium burning cross sections from chiral NN+3N forces
- This will aid in solving long-standing problems in stellar nucleosynthesis
- These developments are also allowing to further expose and will help overcome deficiencies in chiral NN+3N forces