SAN DIEGO STATE UNIVERSITY

Scattering and reactions in a shell-model basis

Calvin W. Johnson

with Minh-Loc Bui and Kenneth M. Nollett

Phys. Rev. C **113**, 024004 (2026)

This material is based upon work supported by the U.S. Department of Energy, under Award Numbers DE-NA0004075 and DE-FG02-96ER40985.

INT "Quantum physics of stars" Aug 18, 2026

Scattering in a shell-model basis

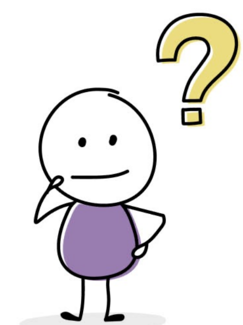
San Diego State University

The team:

Minh-Loc Bui, Postdoc

Kenneth M. Nollett

Calvin W. Johnson



INT "Quantum physics of stars" Aug 18, 2026

San Diego State University

This is not an R-matrix talk!

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey

This is the story of a long journey

This is your quest:

San Diego State University

This is the story of a long journey

This is your quest:
to calculate
n+A scattering *ab initio*

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey

This is your quest:
to calculate
n+A scattering *ab initio*

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey

Do you know
how to compute
n+A scattering *ab initio?*

INT "Quantum physics of stars" Aug 18, 2026

San Diego State University

This is the story of a long journey

Do you know
how to compute
n+A scattering *ab initio?*

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey

Keep your eyes open for n+A scattering *ab initio*…

This is the story of a long journey

If only I knew
how to compute
n+A scattering *ab initio*..

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey

I eat
n+A scattering
for breakfast!

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey

(wait, I'm an experimental method…)

San Diego State University

This is the story of a long journey

It's not easy to compute n+A scattering *ab initio*…

SAN DIEGO STATE UNIVERSITY

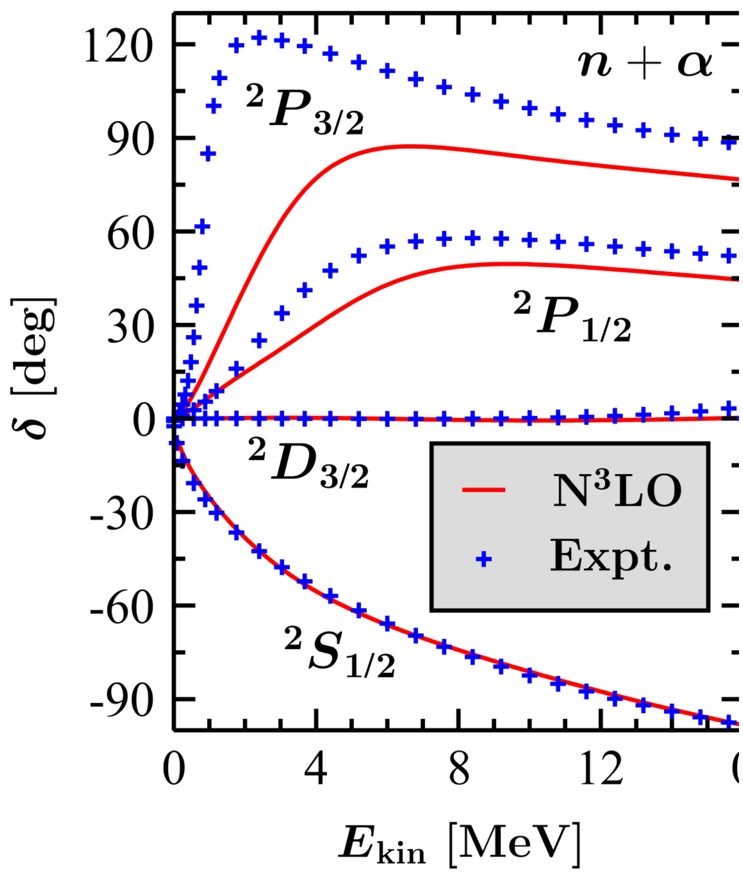
This is the story of a long journey

"White Paper: From bound states to the continuum," CWJ, K. Launey, *et al*, J. Phys. G. **47** 123001 (2020) (from 2018 FRIB Theory alliance workshop)

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey

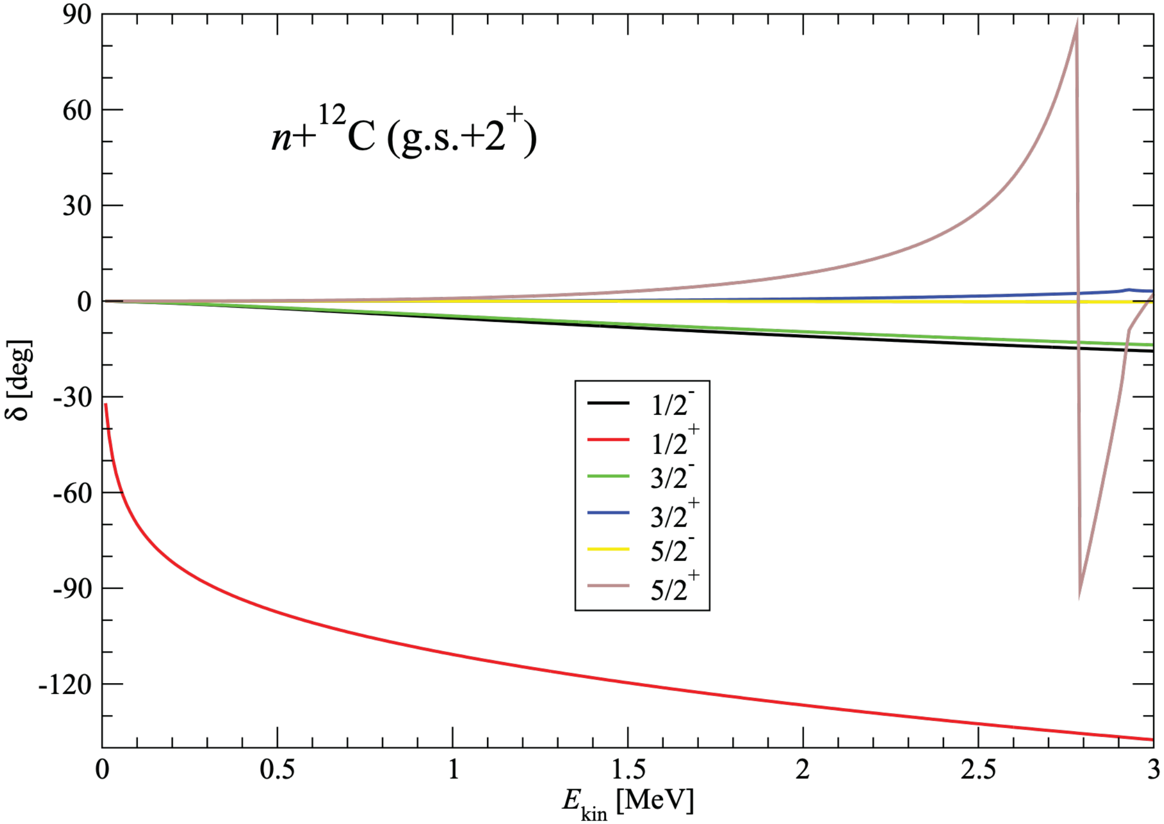


N_{max}=9 dim = 96,340
N_{max}=17 dim = 10 M

PRL **101**, 092501 (2008) see also PRC **79**, 044606 (2009)
NCSM/RGM. Quaglioni and Navratil

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey



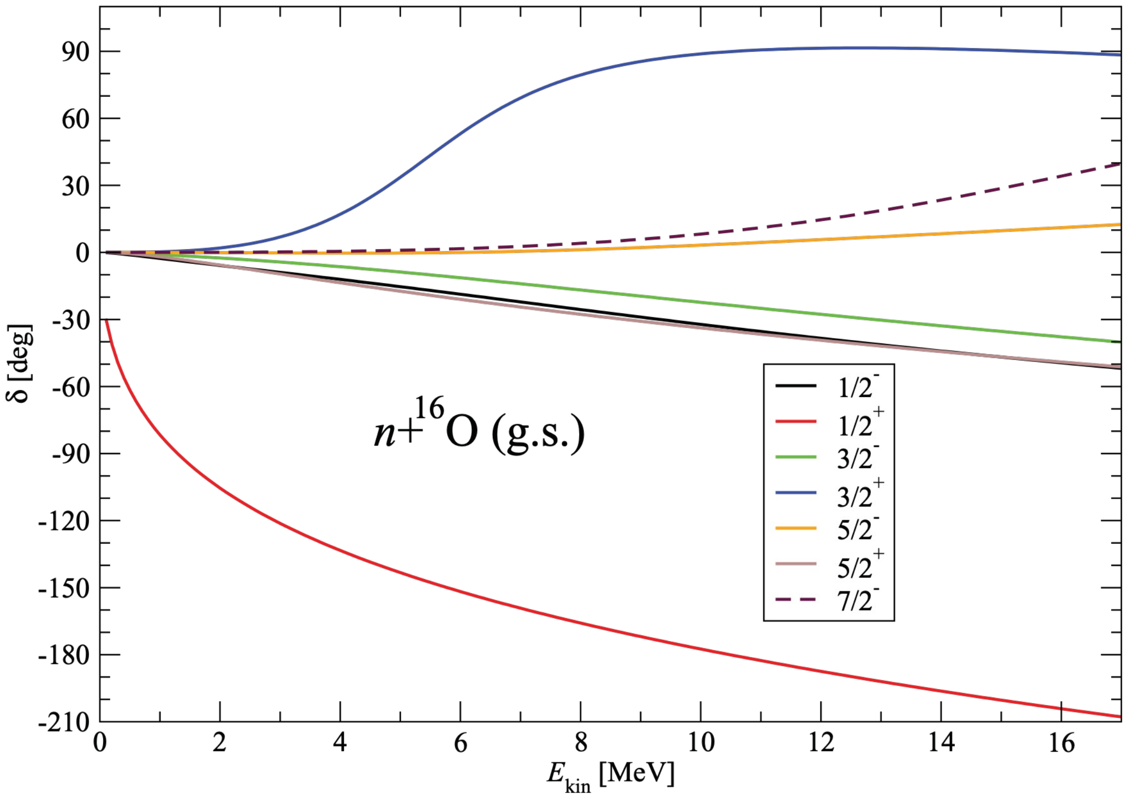
N_{max}=14 dim 7 x 10^{11}

(but reduced using importance truncation)

PRC **82**, 034609 (2010) (see also PRC **109**, 054603 (2024))
NCSM/RGM +IT. (Navratil, Roth, and Quaglioni)

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey



PRC **82**, 034609 (2010)
NCSM/RGM +IT (Navratil, Roth, and Quaglioni)

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY

This is the story of a long journey

$$
\begin{aligned}
&{}_{\mathrm{SD}}\langle\Phi^{J^\pi T}_{\nu' n'}\big|\hat P_{A,A-1}V_{A-2,A-1}\big|\Phi^{J^\pi T}_{\nu n}\rangle_{\mathrm{SD}}\\
&= \frac{1}{2(A-1)(A-2)}\sum_{jj'K\tau}\sum_{n_al_aj_a}\sum_{n_bl_bj_b}\sum_{n_cl_cj_c}\sum_{n_dl_dj_d}\sum_{K_a\tau_aK_{cd}\tau_{cd}}\hat s\hat s'\hat j\hat j'\hat K\hat\tau\hat K_a\hat\tau_a\hat K_{cd}\hat\tau_{cd}(-1)^{I_1'+j'+J+K+j+j_a+j_c+j_d}(-1)^{T_1+\frac12+\tau+T}\\
&\times\begin{Bmatrix} I_1 & \frac12 & s\\ \ell & J & j\end{Bmatrix}\begin{Bmatrix} I_1' & \frac12 & s'\\ \ell' & J & j'\end{Bmatrix}\begin{Bmatrix} I_1 & K & I_1'\\ j' & J & j\end{Bmatrix}\begin{Bmatrix} K_a & K_{cd} & K\\ j' & j & j_a\end{Bmatrix}\begin{Bmatrix} T_1 & \tau & T_1'\\ \frac12 & T & \frac12\end{Bmatrix}\begin{Bmatrix} \tau & \tau_a & \tau_{cd}\\ \frac12 & \frac12 & \frac12\end{Bmatrix}\sqrt{1+\delta_{(n_al_aj_a),(n'\ell'j')}}\sqrt{1+\delta_{(n_cl_cj_c),(n_dl_dj_d)}}\\
&\times\left\langle\left(n'\ell'j'\frac12\right)\left(n_al_aj_a\frac12\right)K_{cd}\tau_{cd}\middle|V\middle|\left(n_dl_dj_d\frac12\right)\left(n_cl_cj_c\frac12\right)K_{cd}\tau_{cd}\right\rangle\\
&\times{}_{\mathrm{SD}}\langle A-1\,\alpha_1'I_1'T_1'|||\left(\left(a^\dagger_{n\ell j\frac12}a^\dagger_{n_al_aj_a\frac12}\right)^{(K_a\tau_a)}\left(\tilde a_{n_cl_cj_c\frac12}\tilde a_{n_dl_dj_d\frac12}\right)^{(K_{cd}\tau_{cd})}\right)^{(K\tau)}|||A-1\,\alpha_1I_1T_1\rangle_{\mathrm{SD}}.
\end{aligned}
\qquad (52)
$$

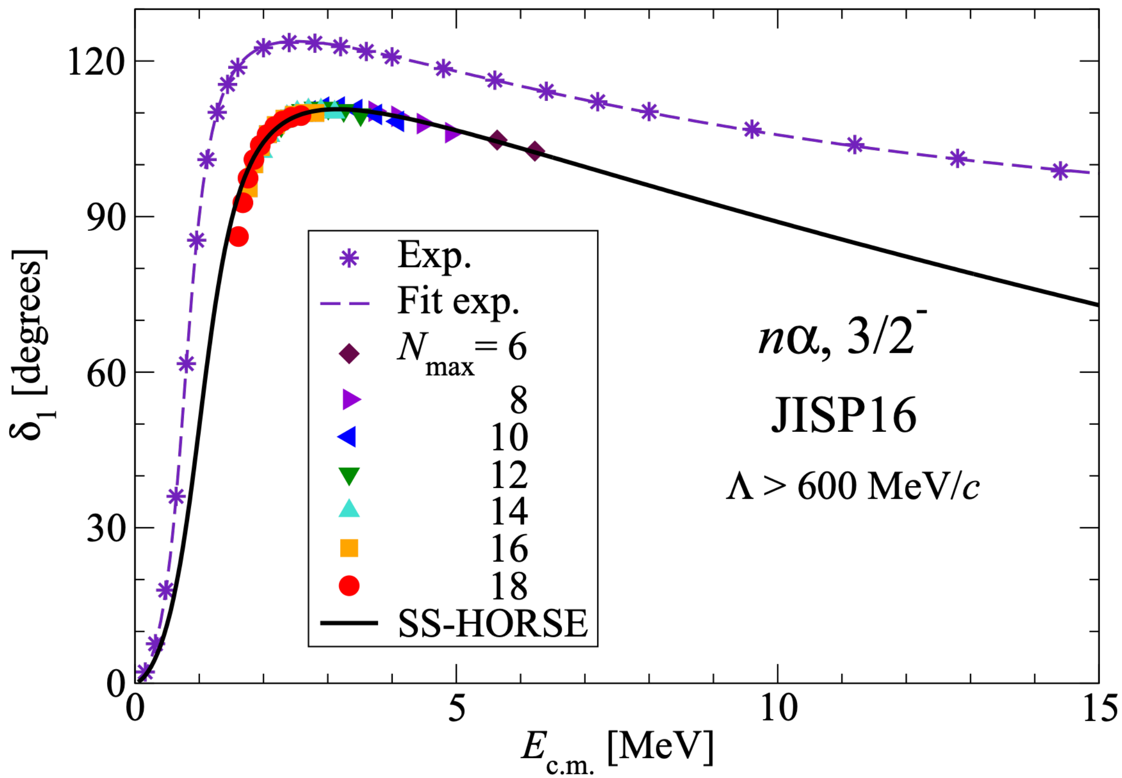
A little piece of the NCSM/RGM formalism

PRL **101**, 092501 (2008) see also PRC **79**, 044606 (2009)
NCSM/RGM. (Quaglioni and Navratil)

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY

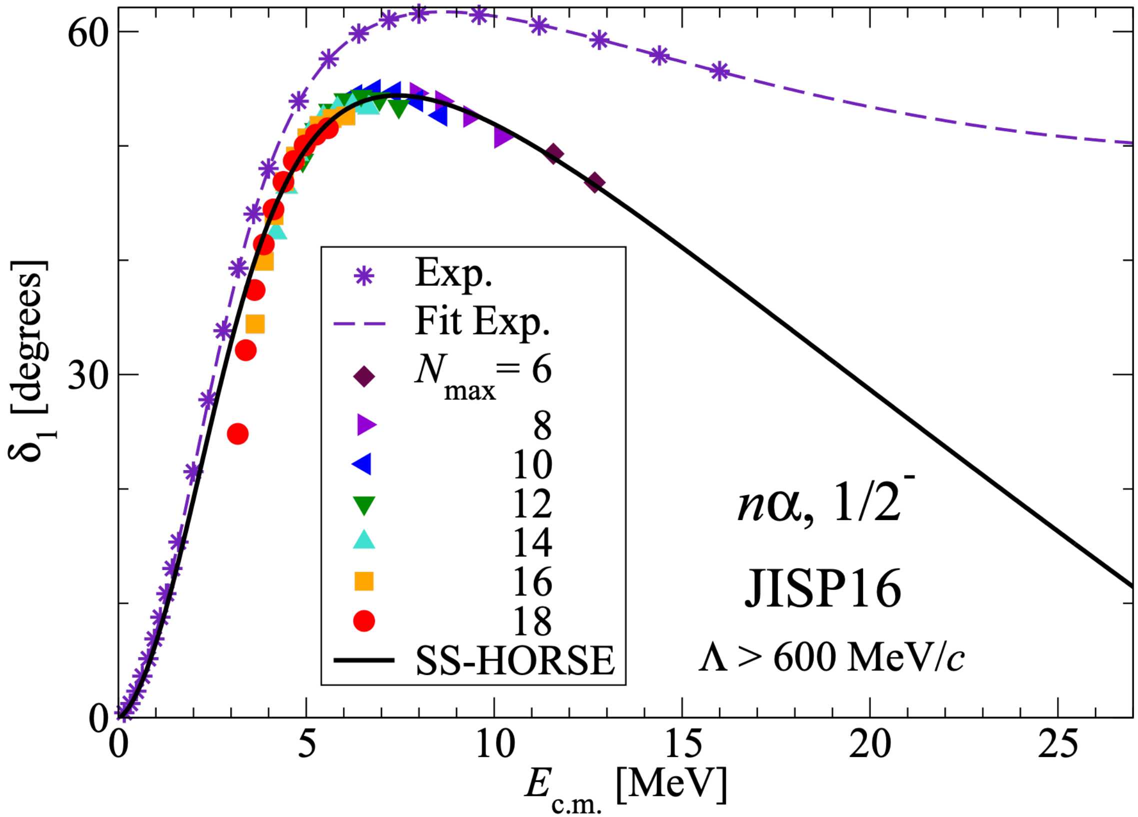
This is the story of a long journey



N_{max}=6 dim = 3,944
N_{max}=18 dim = 643M

PRC **94**, 064320 (2016), Shirokov, Mazur, Mazur, Vary
“SS-HORSE” a variant of J-matrix

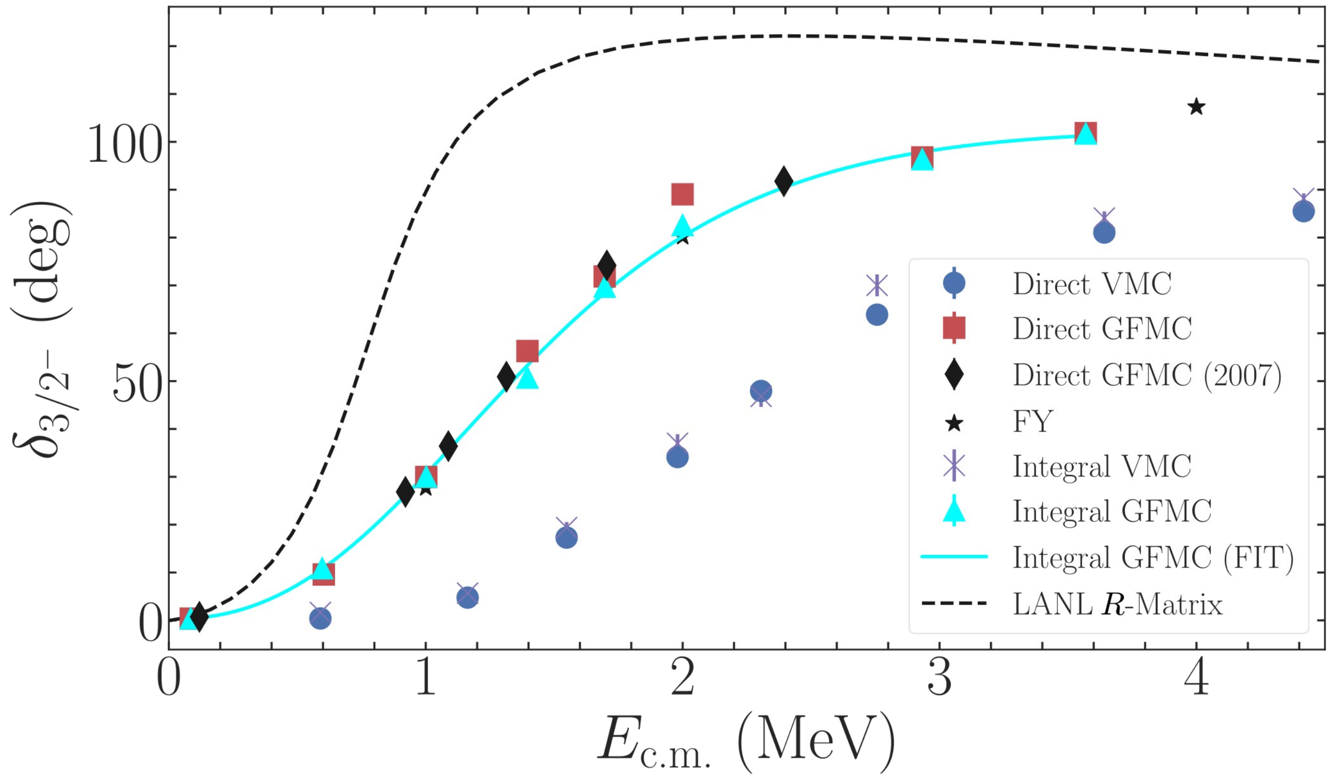
This is the story of a long journey



N_{max}=6 dim = 3,944
N_{max}=18 dim = 643M

PRC **94**, 064320 (2016) Shirokov, Mazur, Mazur, Vary
"SS-HORSE" a variant of J-matrix

This is the story of a long journey

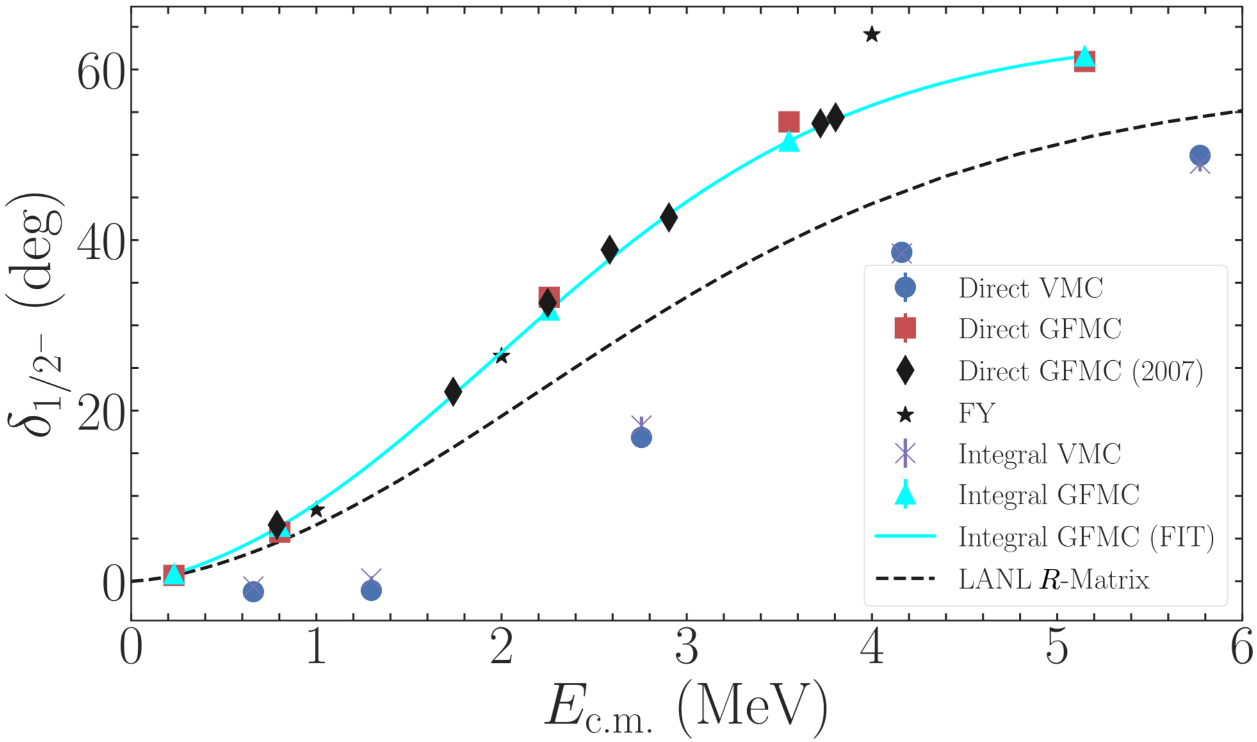


PRC **112**, 014008 (2025) Flores, Nollett, Piarulli
GFMC integral relation in coordinate space

Scattering in a shell-model basis

This is the story of a long journey

SAN DIEGO STATE UNIVERSITY



PRC **112**, 014008 (2025). Flores, Nollett, Piarulli
GFMC integral relation in coordinate space

INT "Quantum physics of stars" Aug 18, 2026

SAN DIEGO STATE UNIVERSITY

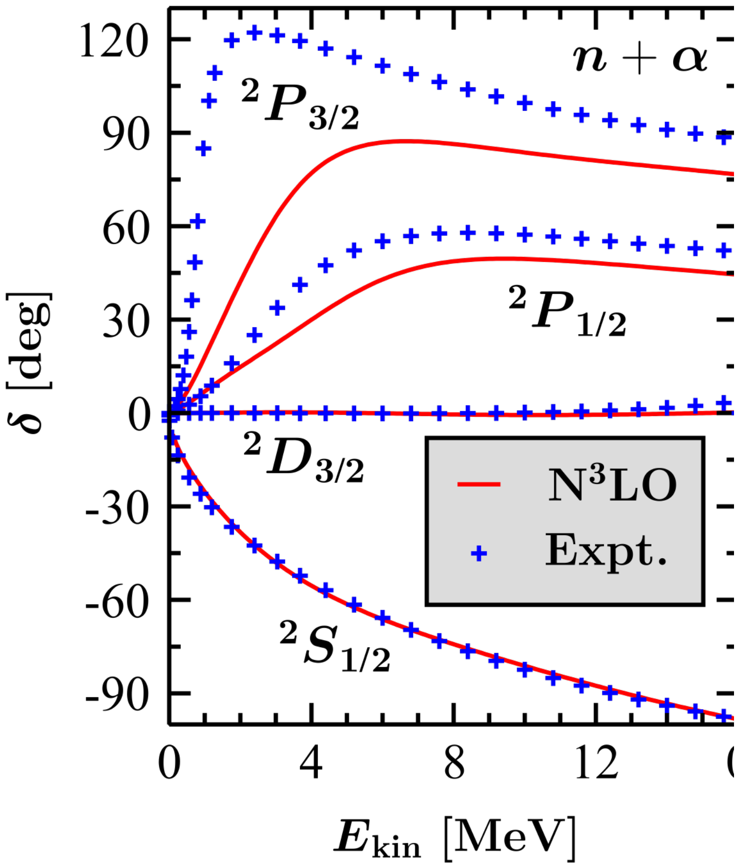
The goal of the project

To develop and improve scattering and reaction methods;

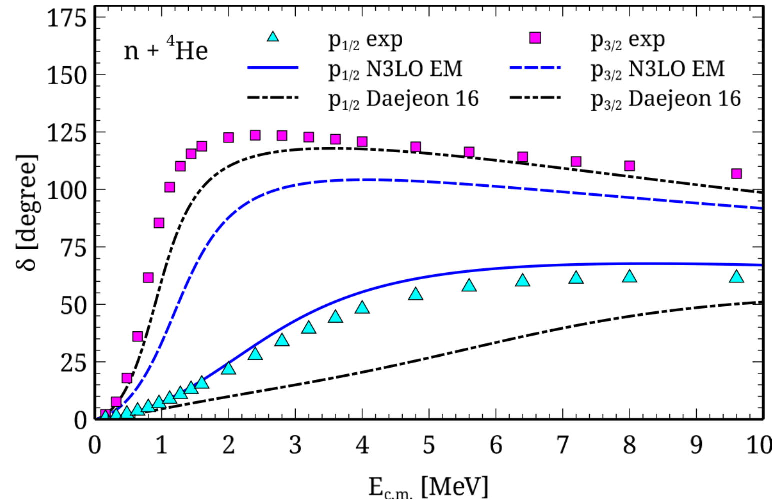
Spoiler alert!

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY



N_{max}=9 dim = 96,340
N_{max}=17 dim = 10 M

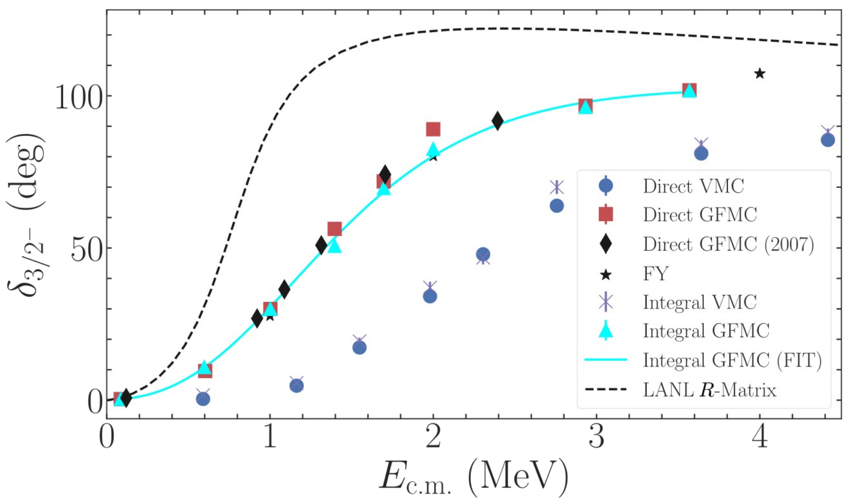


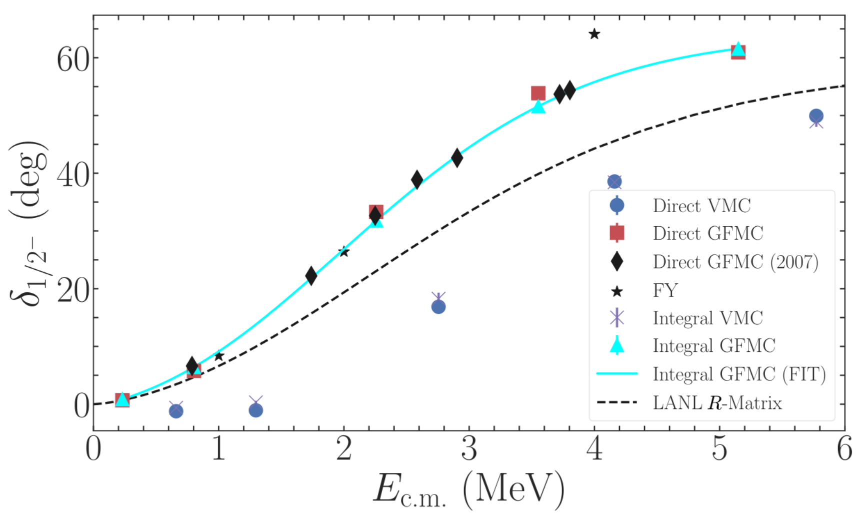
Our work
Dim = 6

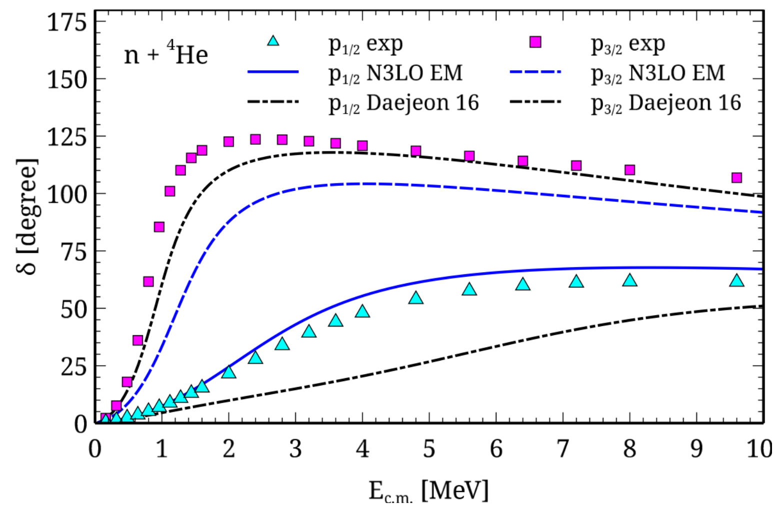
Scattering in a shell-model basis

San Diego State University

GFMC



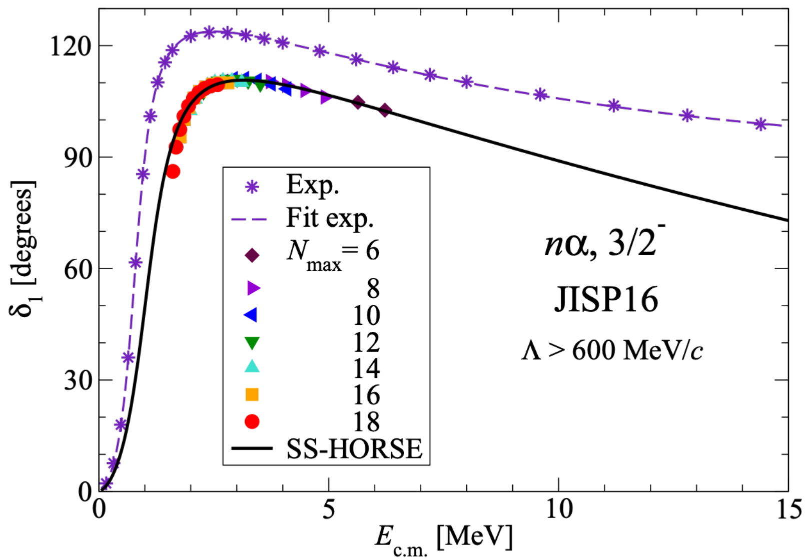


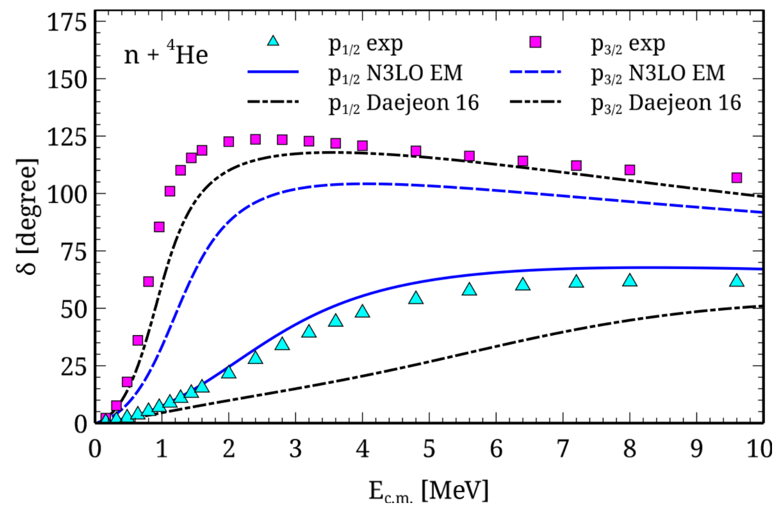


Our work
Dim = 6

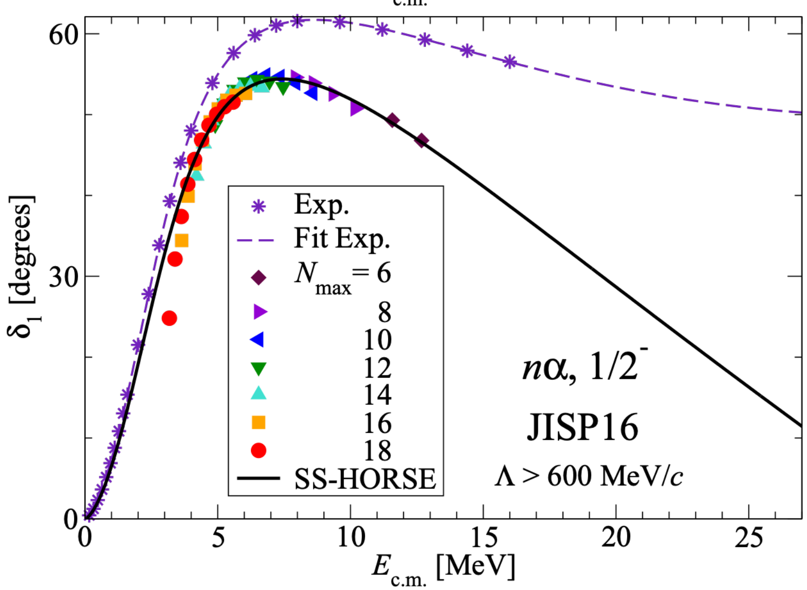
Scattering in a shell-model basis

San Diego State University



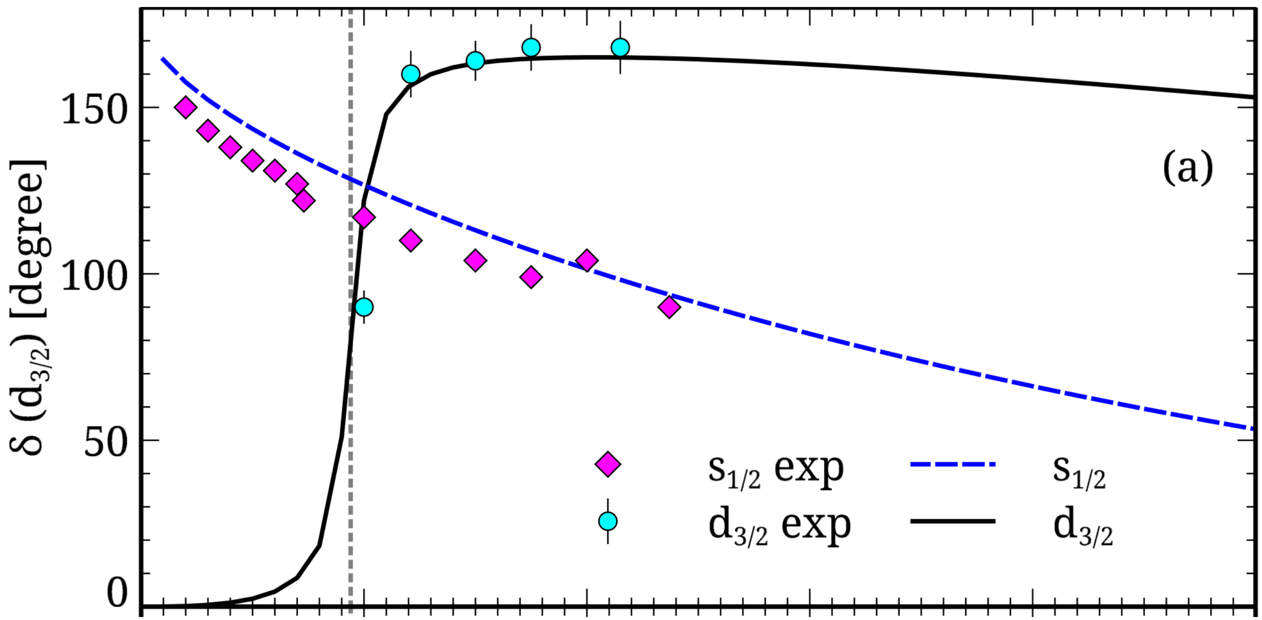


Our work
Dim = 6



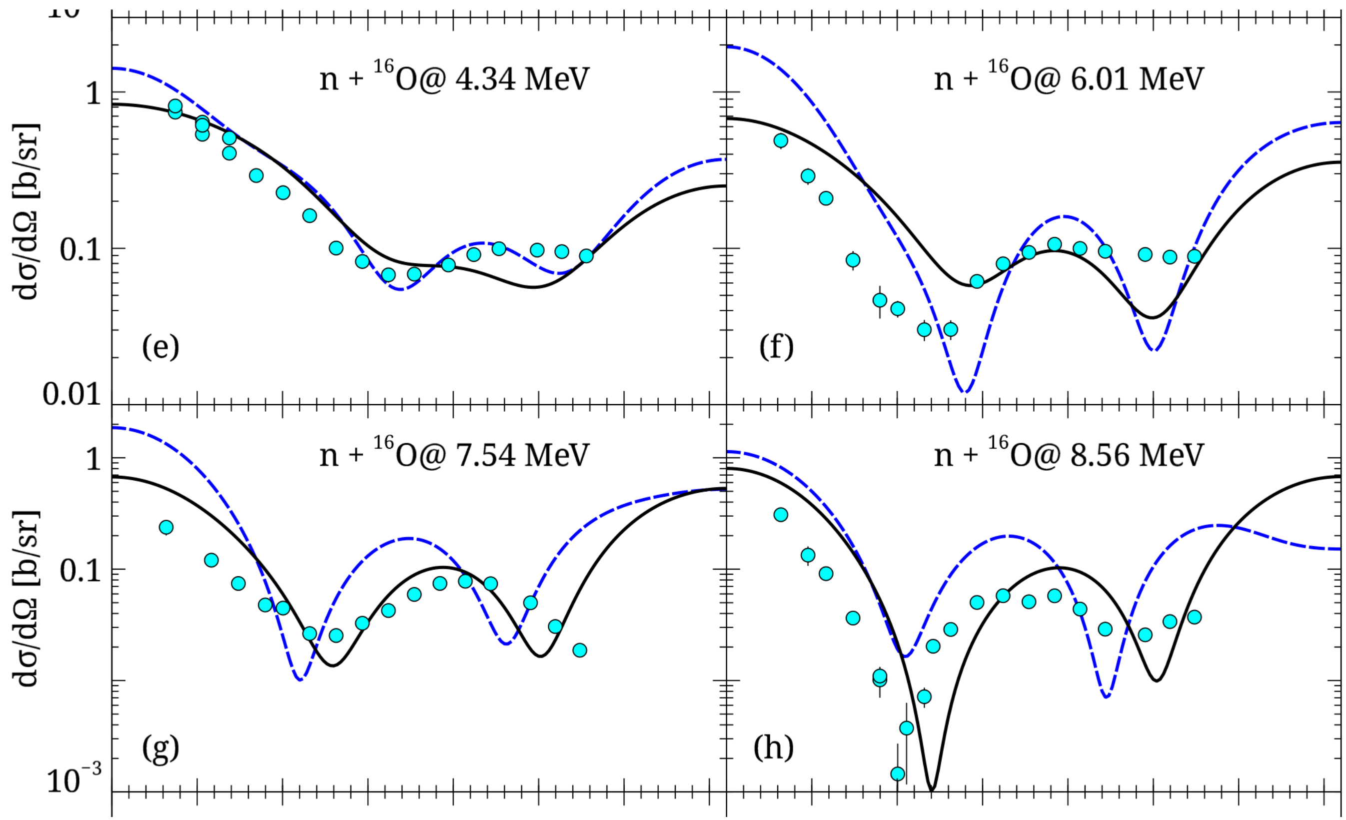
SS-HORSE
N_{max}=6 dim = 3,944
N_{max}=18 dim = 643M

Scattering in a shell-model basis



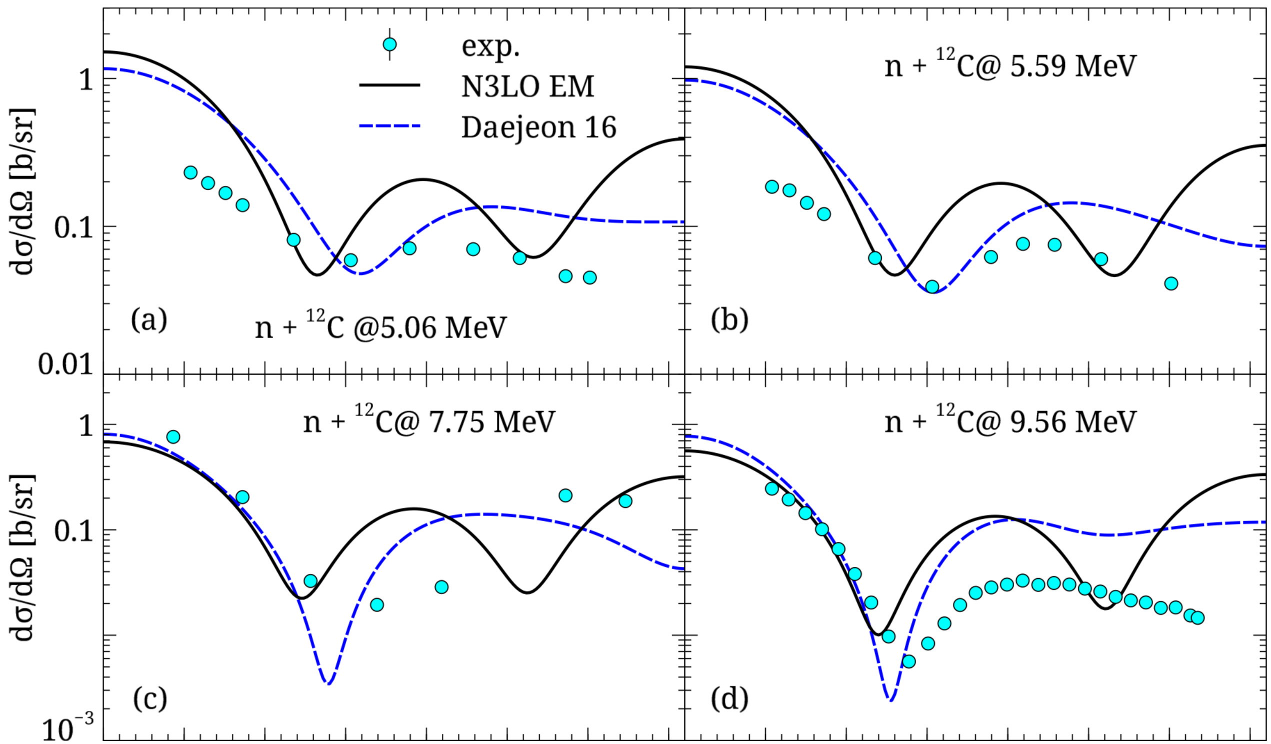
n+^{16}O

n+^{16}O



n + ^{16}O@ 4.34 MeV
n + ^{16}O@ 6.01 MeV
n + ^{16}O@ 7.54 MeV
n + ^{16}O@ 8.56 MeV
(e)
(f)
(g)
(h)
dσ/dΩ [b/sr]
dσ/dΩ [b/sr]
1
0.1
0.01
1
0.1
10^{-3}

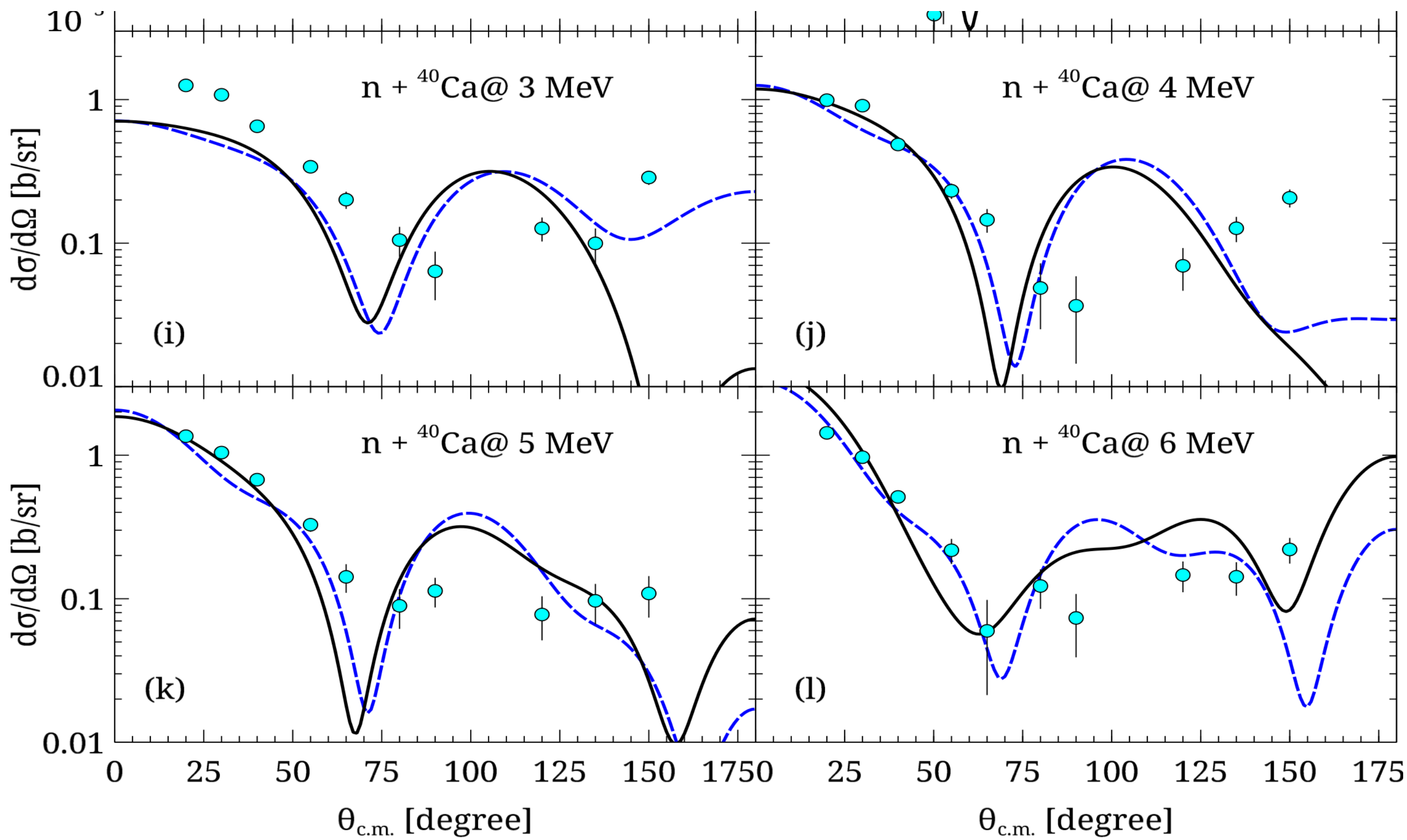
Scattering in a shell-model basis



$n+^{12}C$

GO STATE
RSITY

n+^{40}Ca



The goal of the project

To develop and improve scattering and reaction methods;

Scattering connects **asymptotic** behavior to
the **interior** of the target

SAN DIEGO STATE UNIVERSITY

The goal of the project

To develop and improve scattering and reaction methods;

Scattering connects **asymptotic** behavior to
the **interior** of the target

In particular, I am interested in connecting **scattering** to detailed microscopic models of nuclear wave functions, especially the **nuclear shell model** (no-core and valence)

A few words about….

Configuration-interaction shell model

Matrix formalism:
expand in some (many-body) basis

$$\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$$

$$|\Psi\rangle = \sum_\alpha c_\alpha |\alpha\rangle$$

$$H_{\alpha\beta} = \langle\alpha|\hat{\mathbf{H}}|\beta\rangle$$

$$\sum_\beta H_{\alpha\beta} c_\beta = E c_\alpha$$

A few words about....

Configuration-interaction shell model

Matrix formalism:
expand in some (many-body) basis $\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$

$$|\Psi\rangle = \sum_\alpha c_\alpha |\alpha\rangle$$

$$H_{\alpha\beta} = \langle\alpha|\hat{\mathbf{H}}|\beta\rangle$$

$$\sum_\beta H_{\alpha\beta} c_\beta = E c_\alpha$$

Typical basis states: "Slater determinants" built from L^2-integrable functions, such as harmonic oscillator states

Today's work will only be 'trivial' shell-model, but will set the stage for more complicated work.

The goal of the project

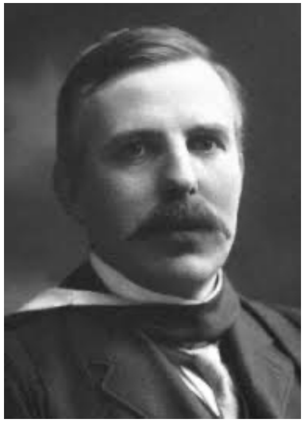
To develop and improve scattering and reaction methods;

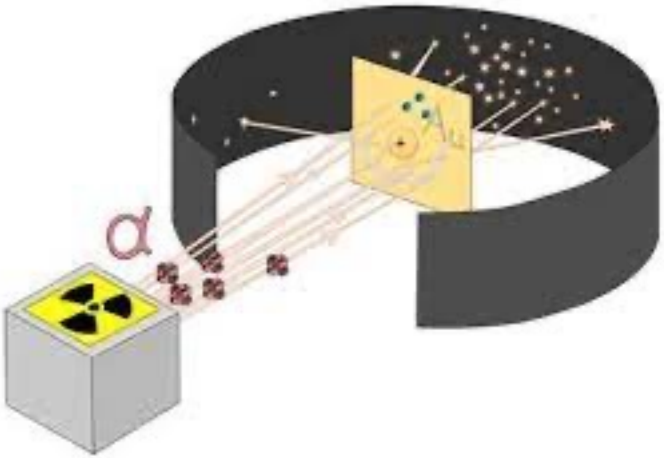
Scattering connects **asymptotic** behavior to the **interior** of the target

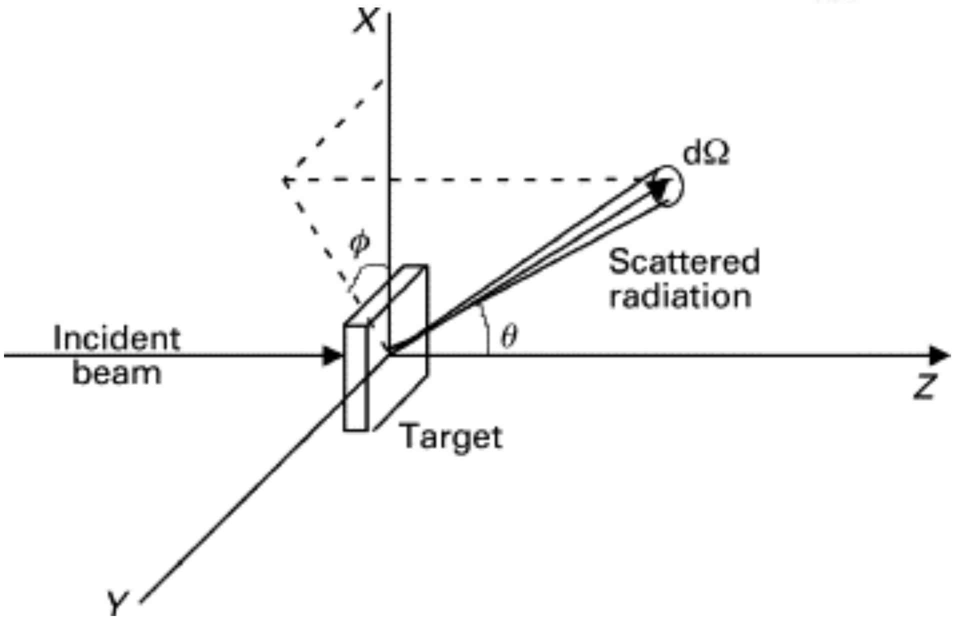
This is a challenge for the shell model:

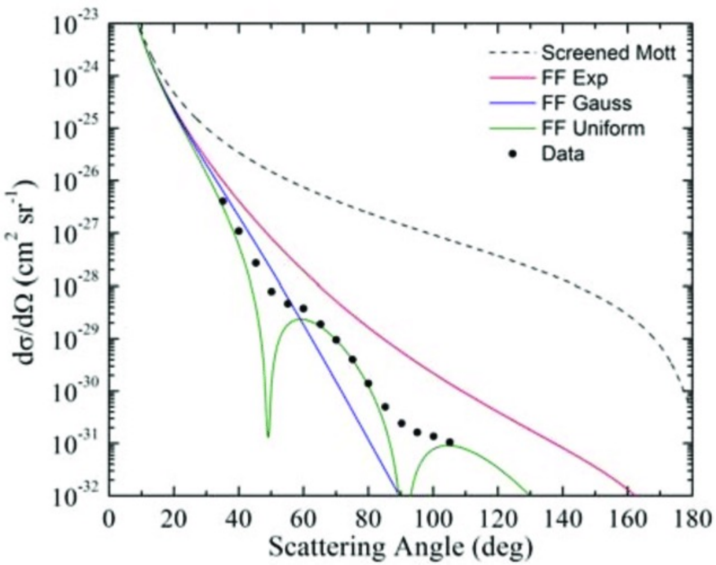
- good description of interior wave function, esp. config. mix.
- poor description of asymptotic behavior

Scattering in a shell-model basis



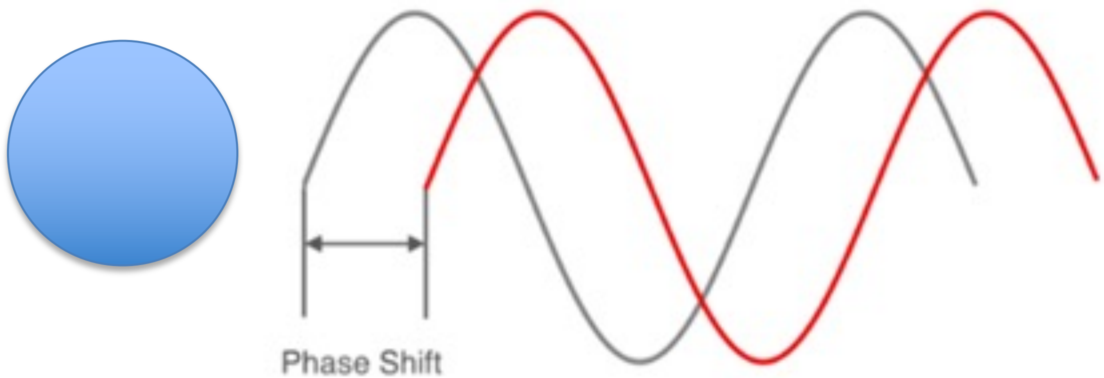






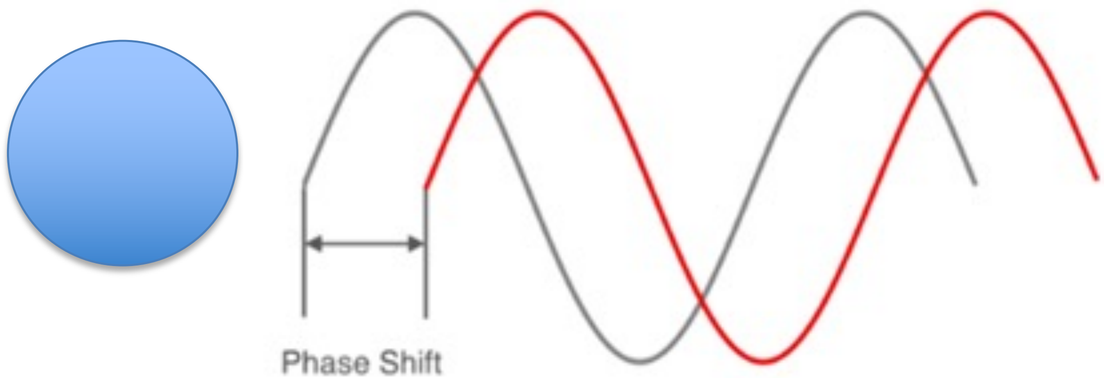
INT "Quantum physics of stars" Aug 18, 2026

Scattering in a shell-model basis

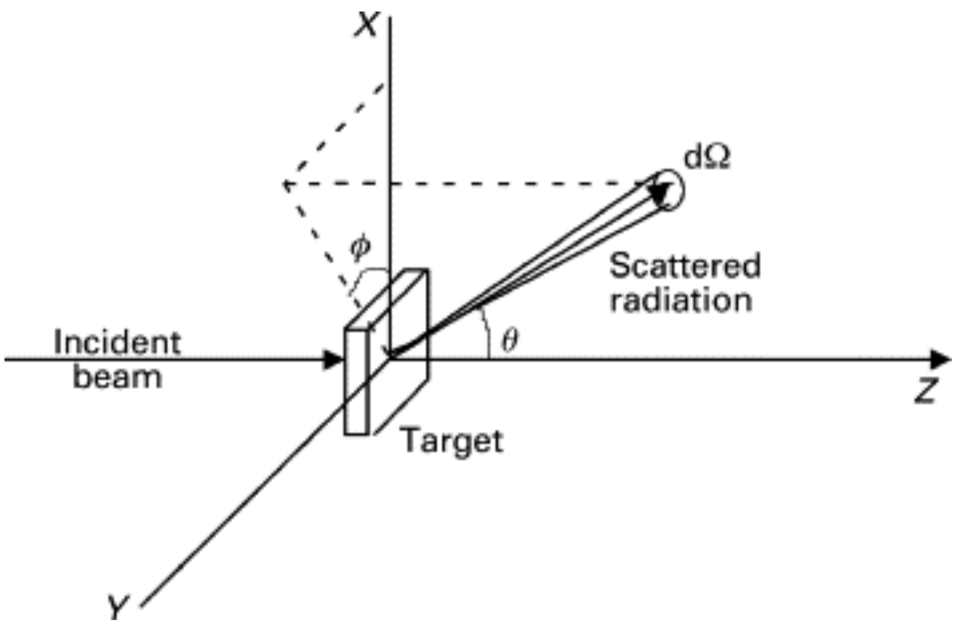


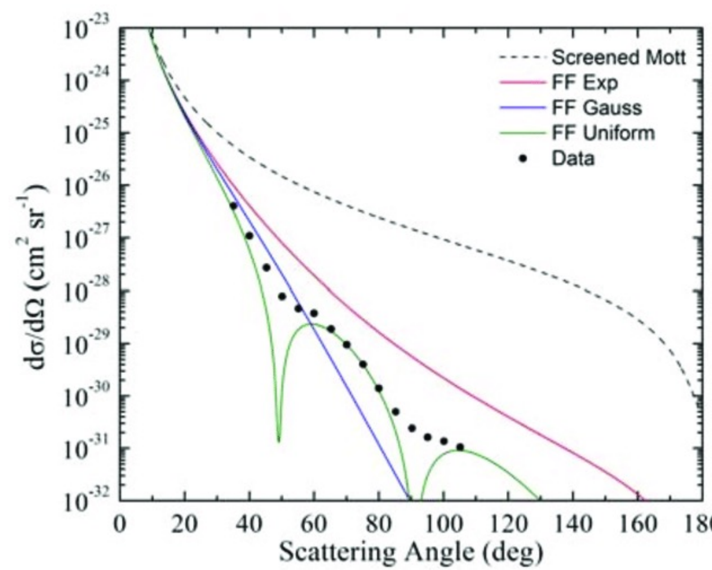
Potential →
Phase shift

Scattering in a shell-model basis

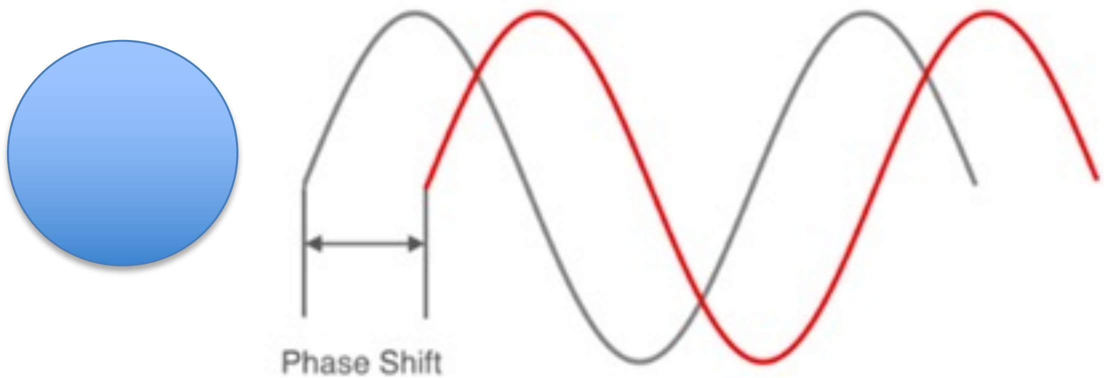


Potential →
Phase shift →
Interference →
Scattering cross-section

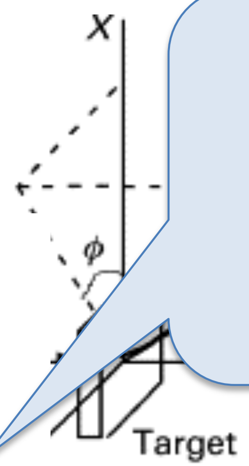


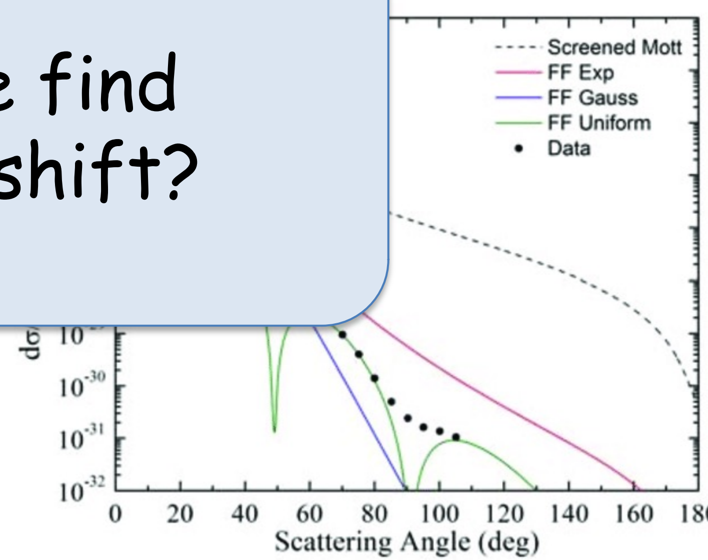


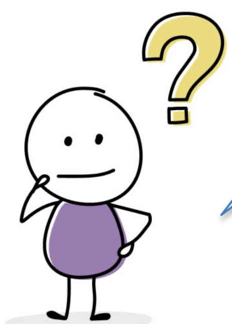
Scattering in a shell-model basis



Potential →
Phase shift →
Interference →
Scattering cross-section



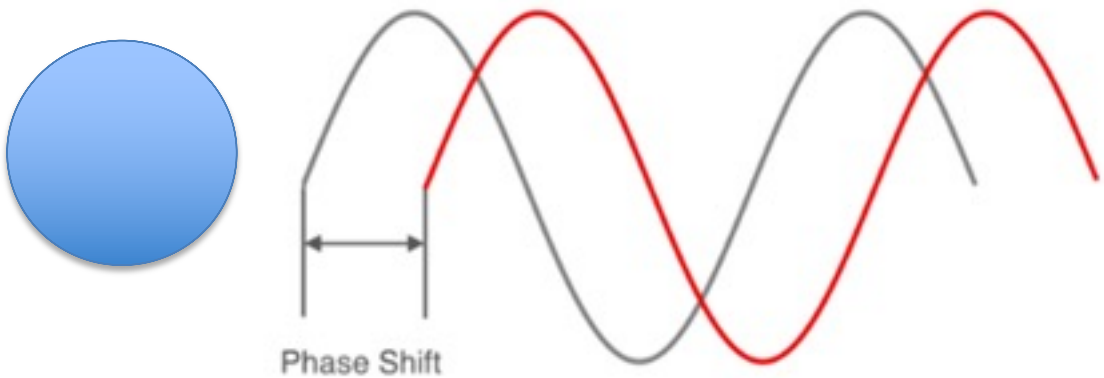


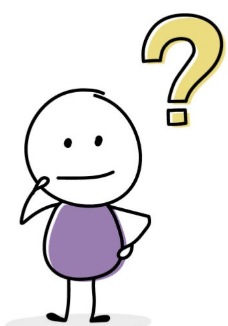


How do we find the phase shift?

Scattering in a shell-model basis

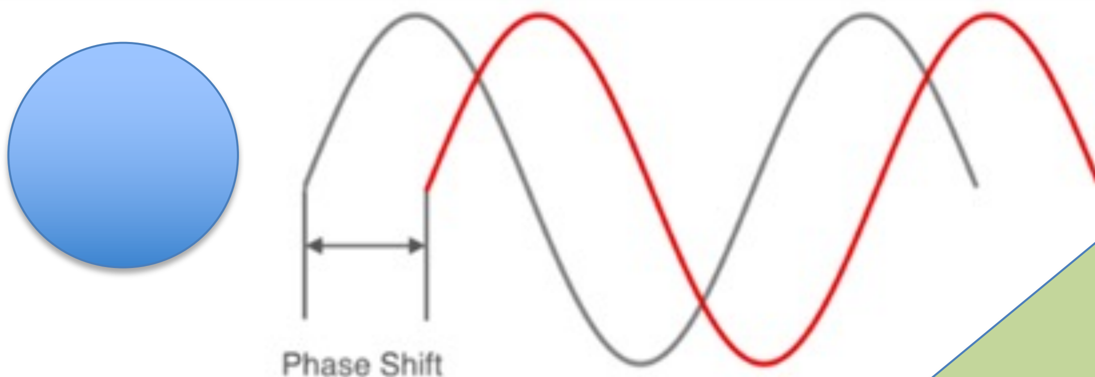
There are **two steps** to computing the phase shift/S-matrix

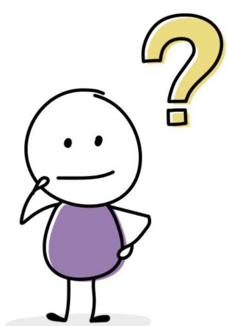




Scattering in a shell-model basis

There are **two steps** to computing the phase shift/S-matrix



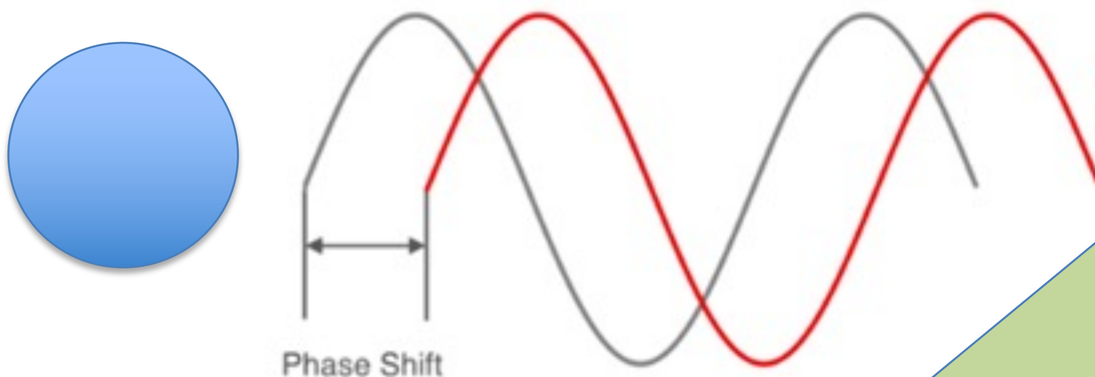


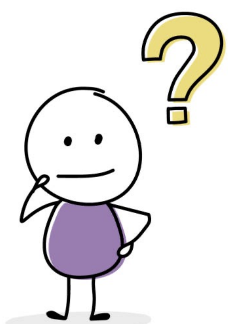
First, generate the scattered state

Scattering in a shell-model basis

San Diego State University

There are **two steps** to computing the phase shift/S-matrix





First, generate the scattered state

Second, extract phase shift/S-matrix

Standard

Scattering State basis

Coordinate or momentum space

↓

Extract phase shift/ S-matrix

Matching

SAN DIEGO STATE UNIVERSITY

	Standard	Novel
Scattering State basis	Coordinate or momentum space	Oscillator or other L^2-integrable
Extract phase shift/ S-matrix	Matching	Overlap/integral

Scattering in a shell-model basis

San Diego State University

	Standard	Novel
Scattering State basis	Coordinate or momentum space	Oscillator or other L^2-integrable
Extract phase shift/ S-matrix	Matching	Overlap/integral

One can also swap methods

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY

	Standard	Novel
Scattering State basis	Coordinate or momentum space	Oscillator or other L^2-integrable
Extract phase shift/ S-matrix	Matching	Overlap/integral

One can also swap methods

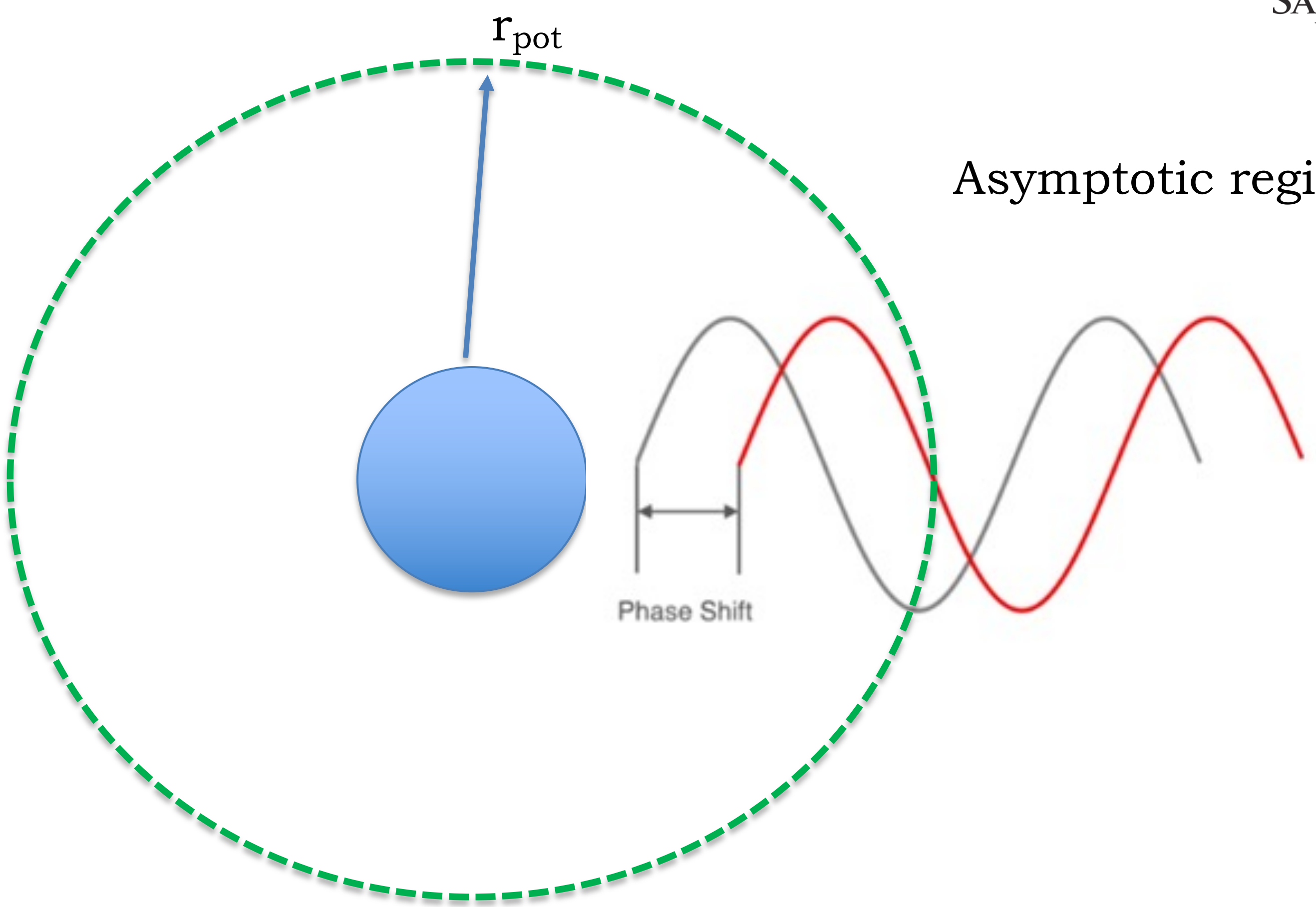
Scattering in a shell-model basis

San Diego State University

	Standard	Novel
Scattering State basis	Coordinate or momentum space	Oscillator or other L^2-integrable
Extract phase shift/ S-matrix	Matching	Overlap/integral

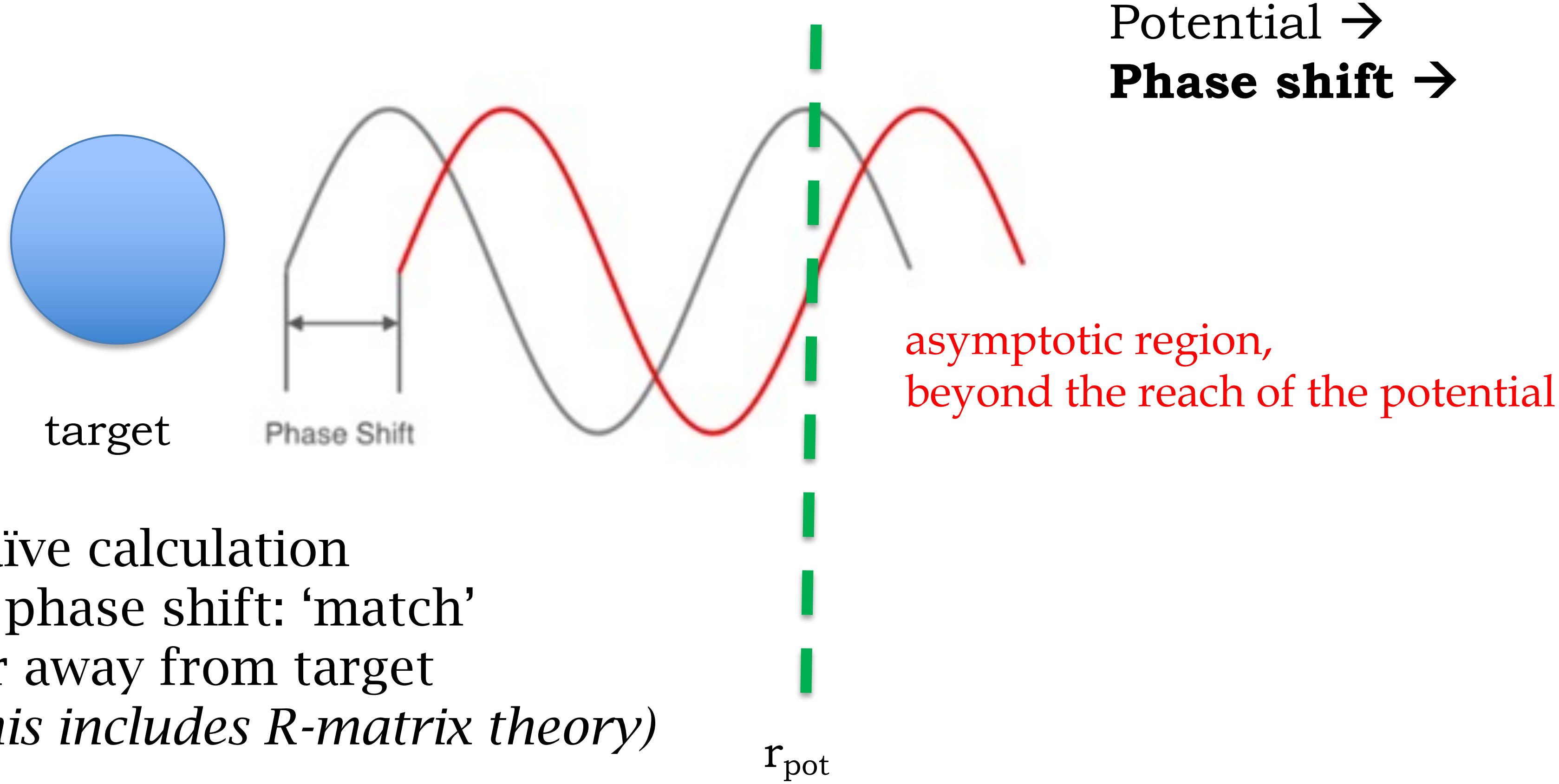
One can also swap methods

Scattering in a shell-model basis



Matching

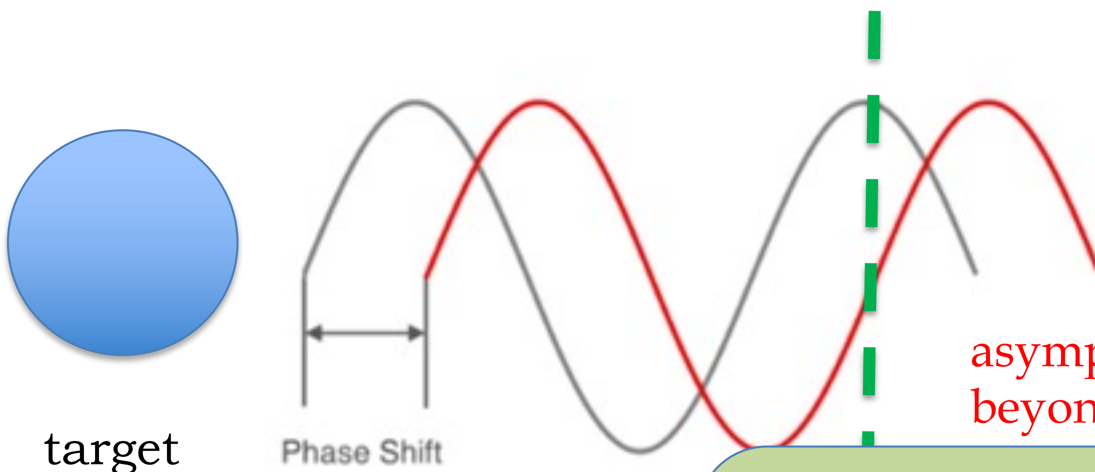
Potential →
Phase shift →



Naïve calculation
of phase shift: 'match'
far away from target
(*this includes R-matrix theory)*

Matching

Potential →
Phase shift →



asymptotic region,
beyond the reach of the potential!

Naïve calculation
of phase shift: 'match'
far away from target
(*this includes R-matrix theory*)

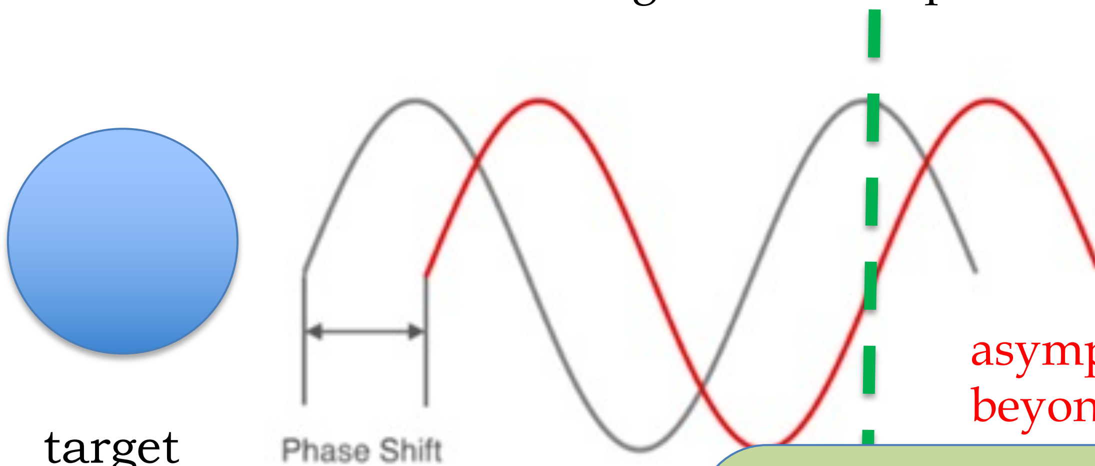
In the asymptotic region, we know the wave function is 'free' (combination of regular and irregular)

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY

$$u_{asymp}(r) = f(r) + \sin\delta \; g(r)$$

regular phase shift irregular $r > r_{pot}$



target

asymptotic region,
beyond the reach of the potential!

Naïve calculation
of phase shift: 'match'
far away from target
(*this includes R-matrix theory*)

In the asymptotic region, we know the wave function is 'free' (combination of regular and irregular)

Scattering in a shell-model basis

$$u_{asymp}(r) = f(r) + \sin\delta \; g(r)$$

regular phase shift irregular $r > r_{pot}$

We 'match' by fitting $u(r)$ to the above for $r > r_{pot}$

or by enforcing some boundary condition, e.g., $u(r_{boundary}) = 0$.

(This will also discretize the continuum)

Scattering in a shell-model basis

San Diego State University

$$u_{asymp}(r) = f(r) + \sin\delta \; g(r)$$

regular phase shift irregular $r > r_{pot}$

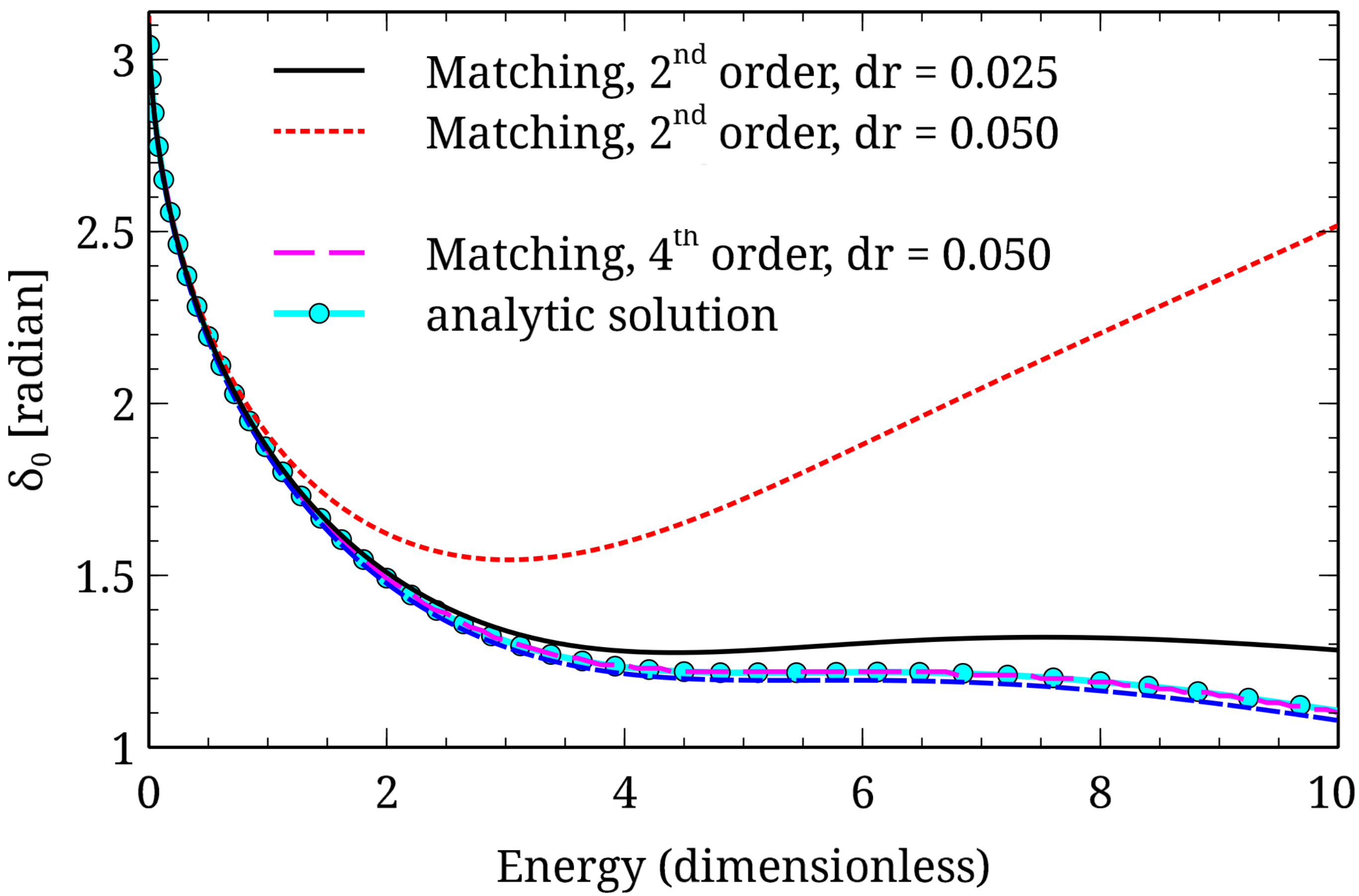
We 'match' by fitting $u(r)$ to the above for $r > r_{pot}$

or by enforcing some boundary condition, e.g., $u(r_{boundary}) = 0$.

(This will also discretize the continuum)

Downsides to matching:
Sensitive to errors,
not always easy to get
'far away' from target

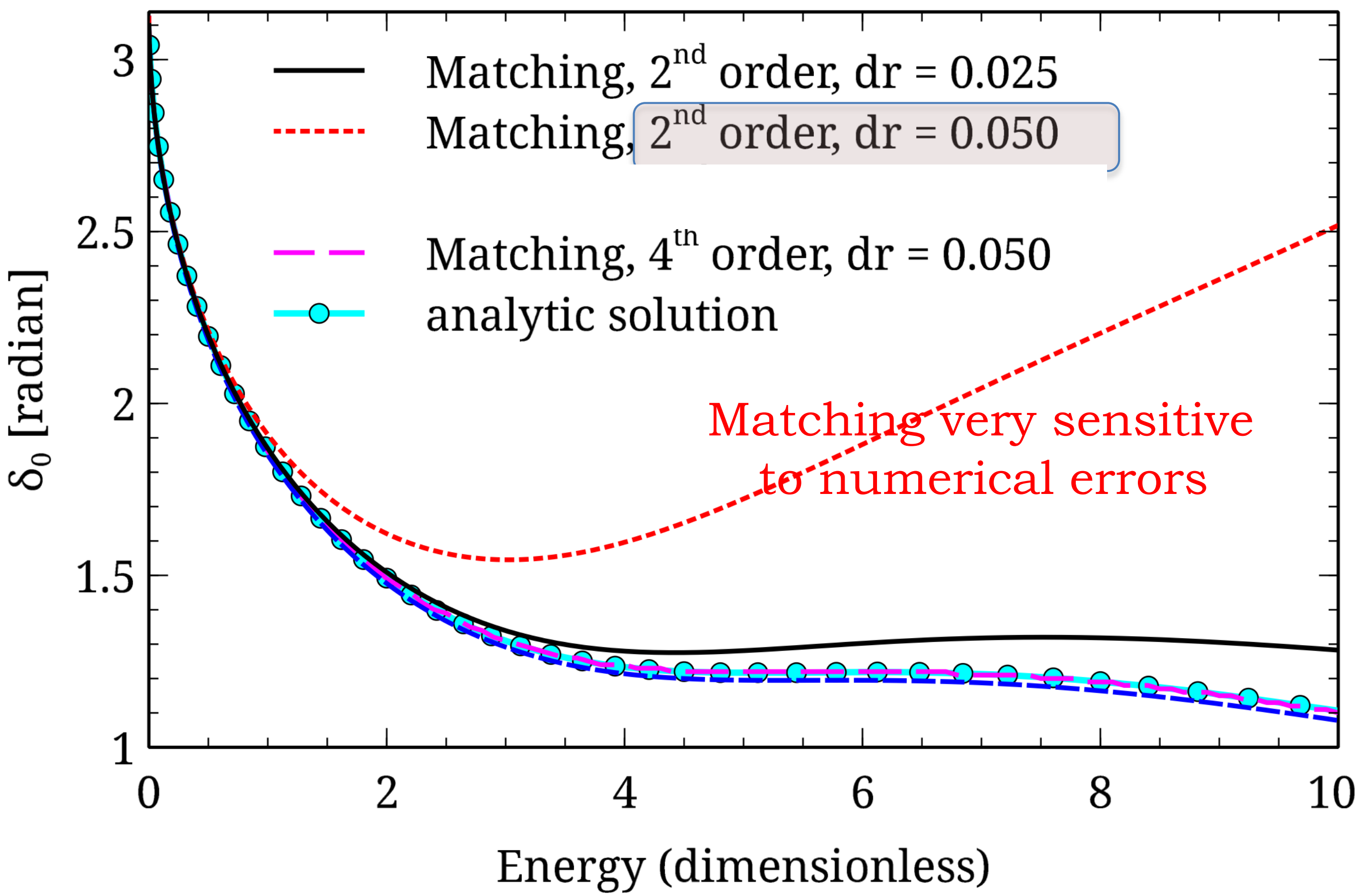
Scattering in a shell-model basis



square well phase shift calculation

well radius = 1 unit

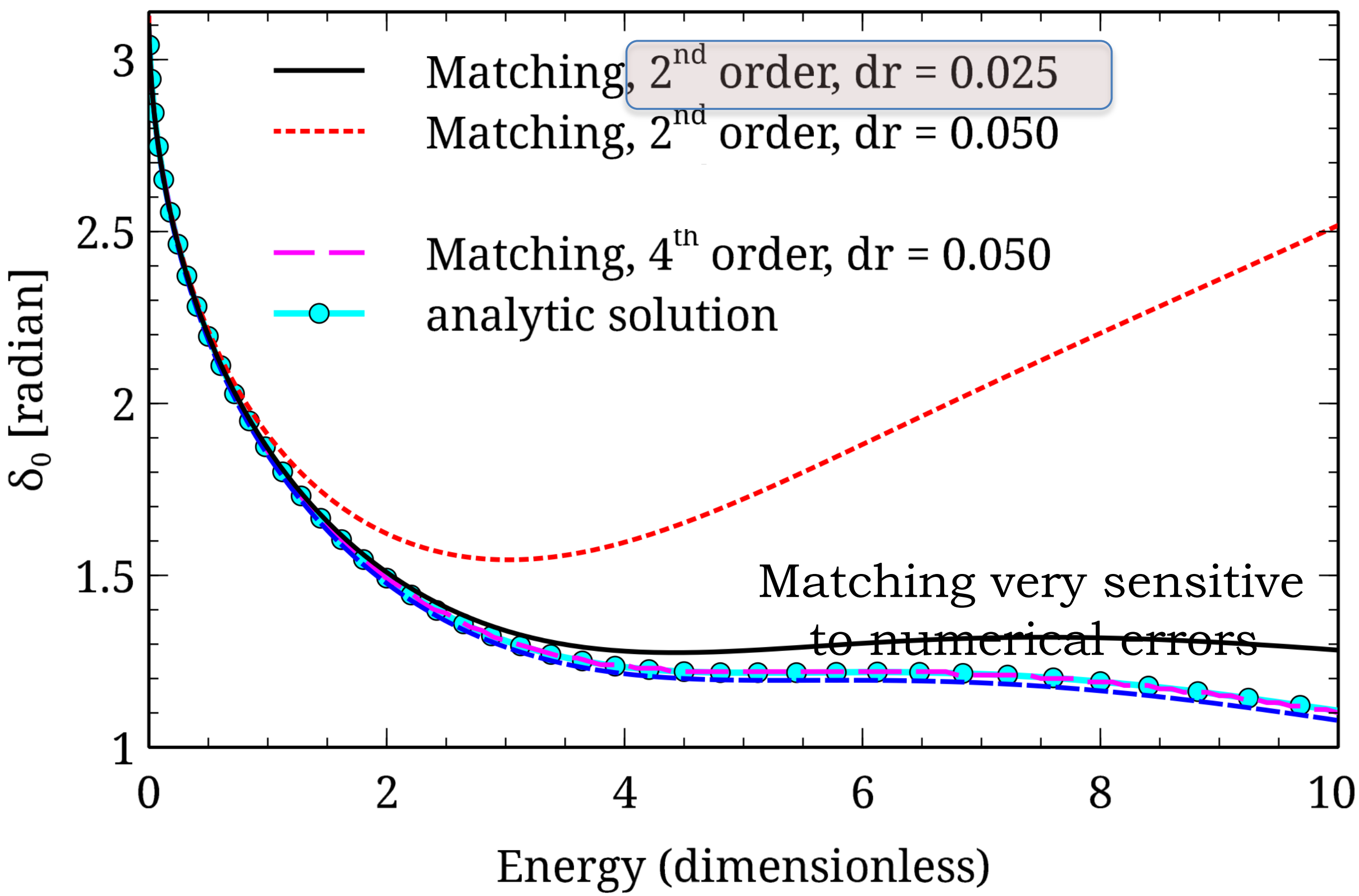
Scattering in a shell-model basis



square well phase shift calculation

well radius = 1 unit

Scattering in a shell-model basis

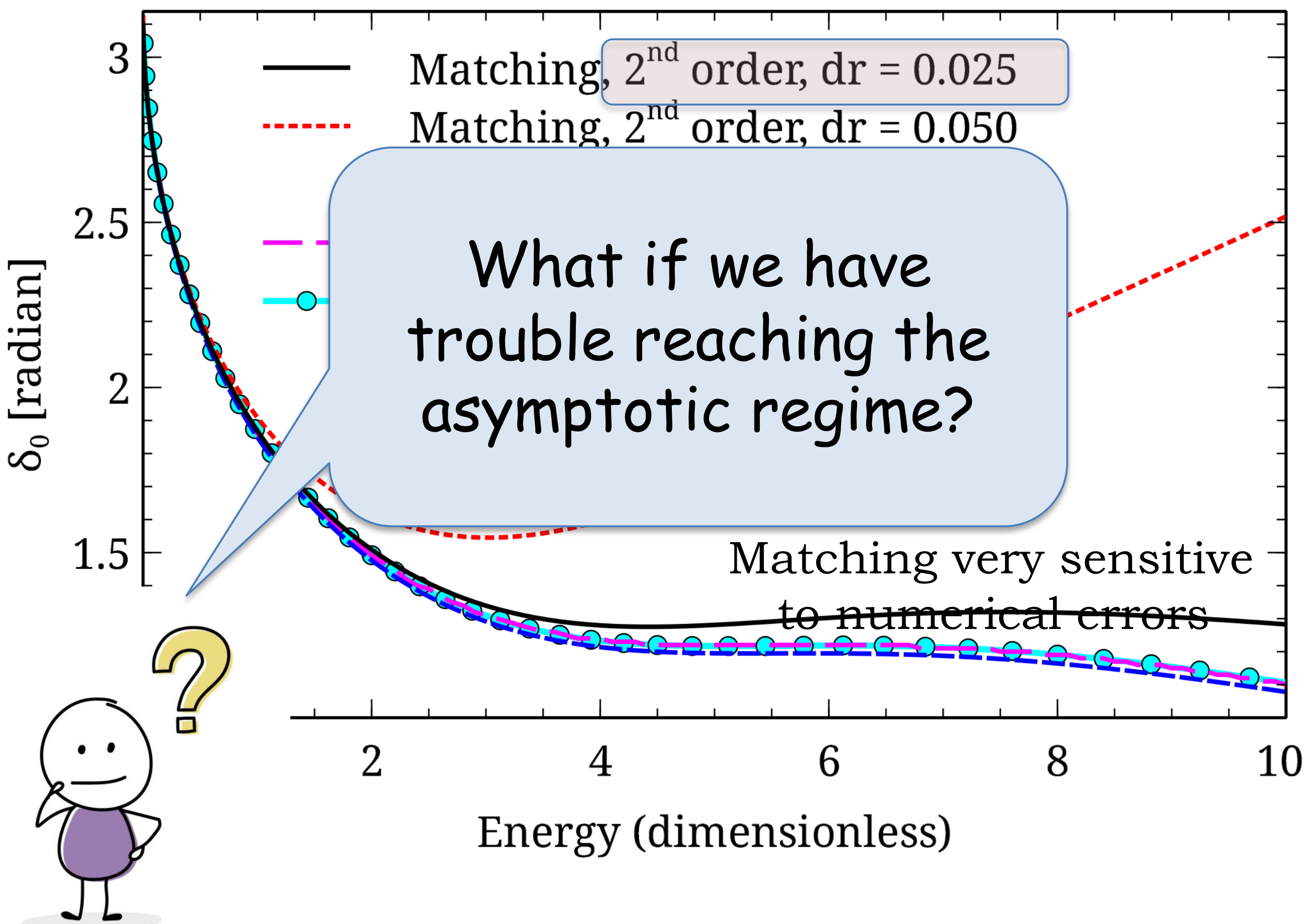


square well phase shift calculation

well radius = 1 unit

Scattering in a shell-model basis

San Diego State University



What if we have trouble reaching the asymptotic regime?

square well phase shift calculation

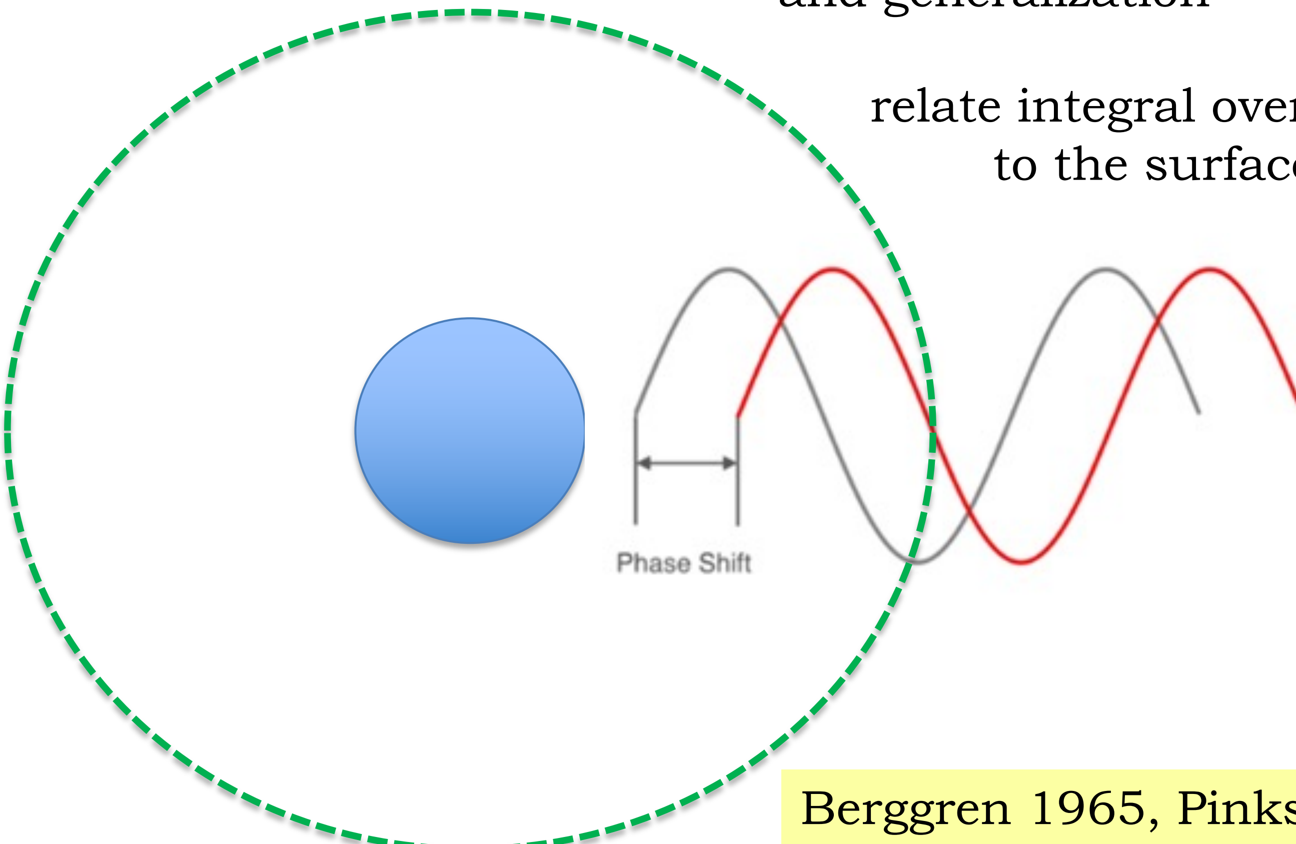
well radius = 1 unit

Math to the rescue!

SAN DIEGO STATE UNIVERSITY

Green's theorem/Stokes' theorem
and generalization

relate integral over volume
to the surface



Berggren 1965, Pinkston & Satchler 1965
Kievsky, et al, PRC **81**, 034002 (2010);
Flores & Nollett, PRC **108**,034001 (2023)

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY

	Standard	Novel
Scattering State basis	Coordinate or momentum space	
Extract phase shift/ S-matrix		Overlap/integral

Math to the rescue!

Kievsky, et al, PRC **81**, 034002 (2010);
Flores & Nollett, PRC **108**, 034001 (2023)
CWJ et al, Phys. Rev. C **113**, 024004 (2026)

Green's theorem/Stokes' theorem and generalization

relate integral over volume to the surface

potential (limits range of integral)

full scattering function

regular free scattering function

$$\tan \delta = - \frac{\int f(r) V(r) u(r) dr}{\int g(r) V(r) u(r) dr + g(0) u'(0) - g'(0) u(0)}$$

irregular free scattering function

correction term (arises from inhomogeneous diff eqn)

Math to the rescue!

"scattering overlap relation" = SOR

Green's theorem/Stokes' theorem and generalization

relate integral over volume to the surface

potential (limits range of integral)

full scattering function

regular free scattering function

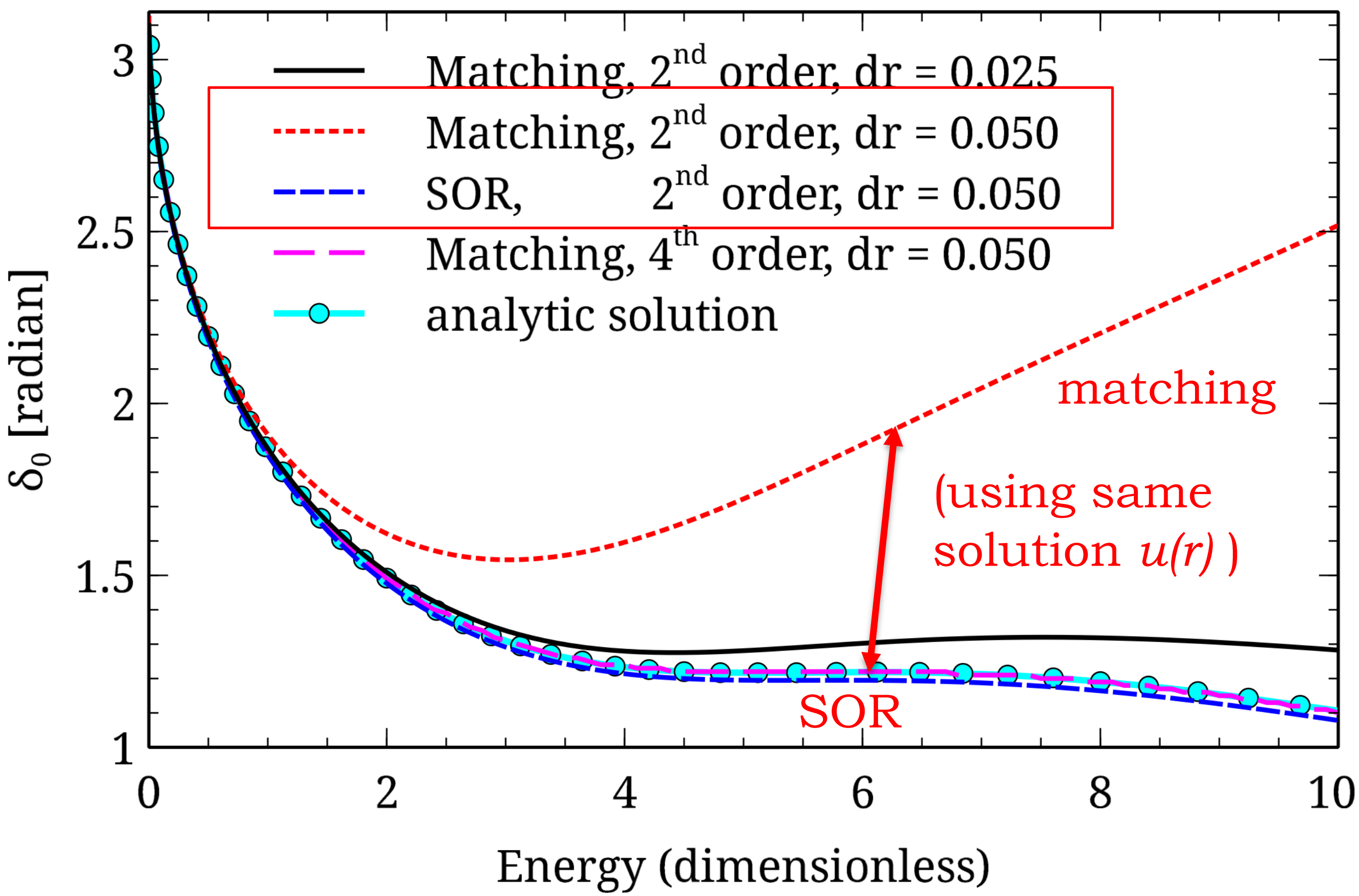
$$\tan\delta = -\frac{\int f(r)V(r)u(r)dr}{\int g(r)V(r)u(r)dr + g(0)u'(0) - g'(0)u(0)}$$

correction term (arises from inhomogeneous diff eqn)

irregular free scattering function

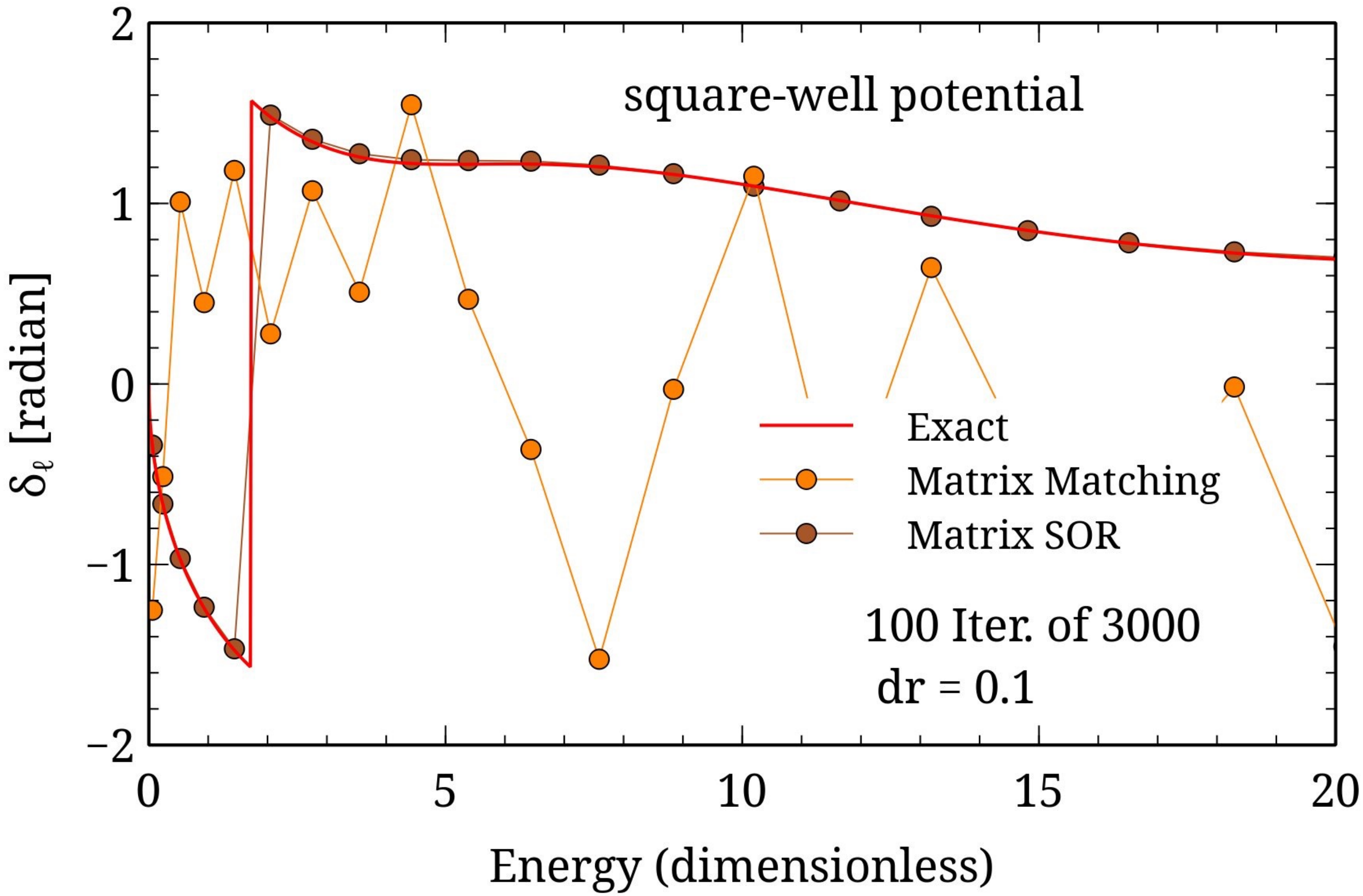
Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY



square well phase shift calculation

Scattering in a shell-model basis

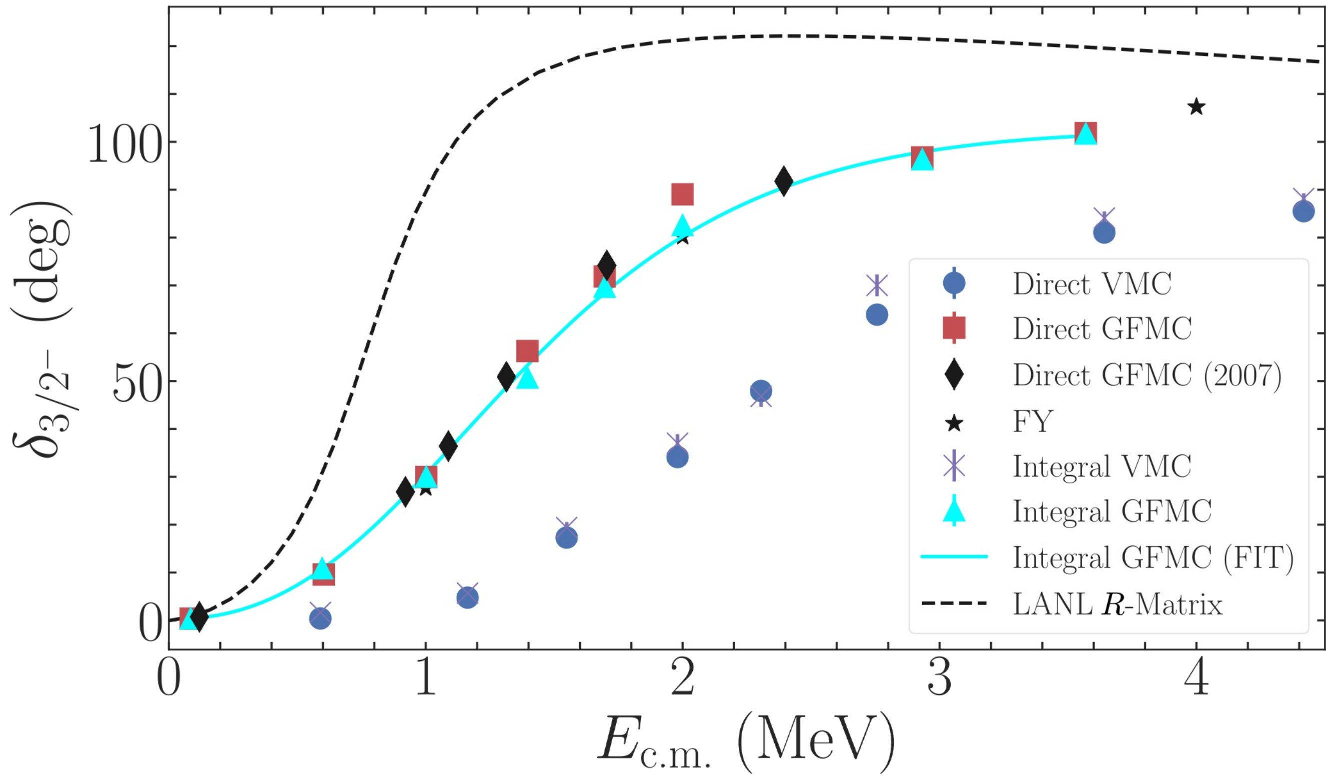


Approx calculation from Lanczos → Slow to converge at large *r*

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY

Example of coordinate-space overlap



PRC **112**, 014008 (2025) Flores, Nollett, Piarulli
GFMC integral relation in coordinate space

Scattering in a shell-model basis

	Standard	Novel
Scattering State basis	Coordinate or momentum space	
Extract phase shift/ S-matrix		Overlap/integral

The story so far....

Matching extracts the phase shift directly at large distance…

Overlap relations use an integral (overlap) over the interior to deduce the phase shift at large distance…

…and is often much more accurate than matching.

SAN DIEGO STATE UNIVERSITY

The goal of the project

To develop and improve scattering and reaction methods;

in particular to develop and apply analogs of ‘overlap integrals’ to shell-model calculations of scattering in many-body systems

This requires modeling scattering with finite basis functions (e.g., harmonic oscillator basis functions)

The challenge

Computing scattering in a shell –model basis is not obvious.

- One can represent scattering states in a harmonic oscillator basis ("J-matrix method" Heller & Yamani, PRA **9**, 1201 (1974))
 which is congruent with no-core shell model
Cf. Shirokov *et al*, PRC **94**, 064320 (2016)

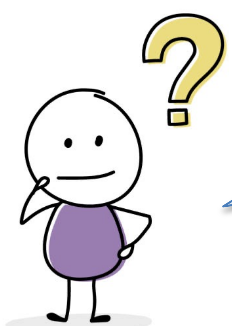
SAN DIEGO STATE UNIVERSITY

The challenge

Computing scattering in a shell –model basis is not trivial.

- One can represent scattering states in a harmonic oscillator basis

(“J-matrix method”) which is congruent with no-core shell model
Cf. Shirokov *et a*



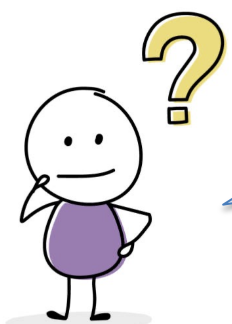
SAN DIEGO STATE UNIVERSITY

The challenge

Computing scattering in a shell –model basis is not trivial.

- One can represent scattering states in a harmonic oscillator basis (“J-matrix method”) which is congruent with no-core shell model

Cf. Shirokov *et a*



Wait, you can represent scattering states in a harmonic oscillator basis?

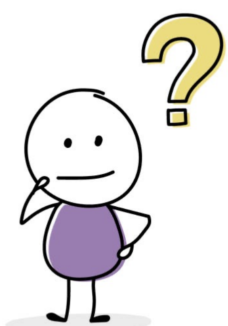
Yes!

Scattering in a shell-model basis

San Diego State University

Consider the free (s-wave) regular function.
We can expand in a basis…

$$f(k,r) = \sin(kr) = \sum_n f_n(k)\, \phi_n(r)$$



Scattering in a shell-model basis

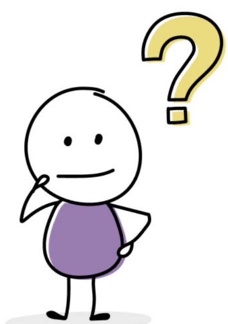
SAN DIEGO STATE UNIVERSITY

Consider the free (s-wave) regular function.
We can expand in a basis…

$$f(k,r) = \sin(kr) = \sum_n f_n(k)\,\phi_n(r)$$

For oscillator basis states, the expansion coefficients f_n are known analytically.

(One can develop a complete theory when the matrix elements of the kinetic energy form a tridiagonal or Jacobi (J) matrix
Heller & Yamani, PRA **9**, 1201 (1974))



Scattering in a shell-model basis

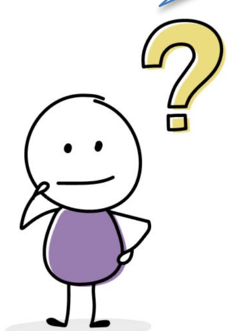
San Diego State University

Consider the free (s-wave) regular function.
We can expand in a basis…

$$f(k,r) = \sin(kr) = \sum f_n(k)\,\phi_n(r)$$

For oscillato … nalytically.

(One can d … trix elements
of the ki … (J) matrix)



Scattering in a shell-model basis

$$T = \begin{pmatrix} T_{00} & T_{01} & 0 & 0 & \cdots & 0 & 0 \\ T_{10} & T_{11} & T_{12} & 0 & \cdots & 0 & 0 \\ 0 & T_{21} & T_{22} & T_{23} & \cdots & 0 & 0 \\ 0 & 0 & T_{32} & T_{33} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & T_{9\,9} & T_{9\,10} \\ 0 & 0 & 0 & 0 & \cdots & T_{10\,9} & T_{10\,10} \end{pmatrix}$$

Tridiagonal or J-matrix form of KE

$$u_{scatt}(r) = \sum_n u_n \, \phi_n(r)$$

Truncation here implies $u_{11} = 0$
→ discretizes continuum

SAN DIEGO STATE UNIVERSITY

The challenge

Computing scattering in a shell –model basis is not trivial.

- One can represent scattering states in a harmonic oscillator basis ("J-matrix method") which is congruent with no-core shell model

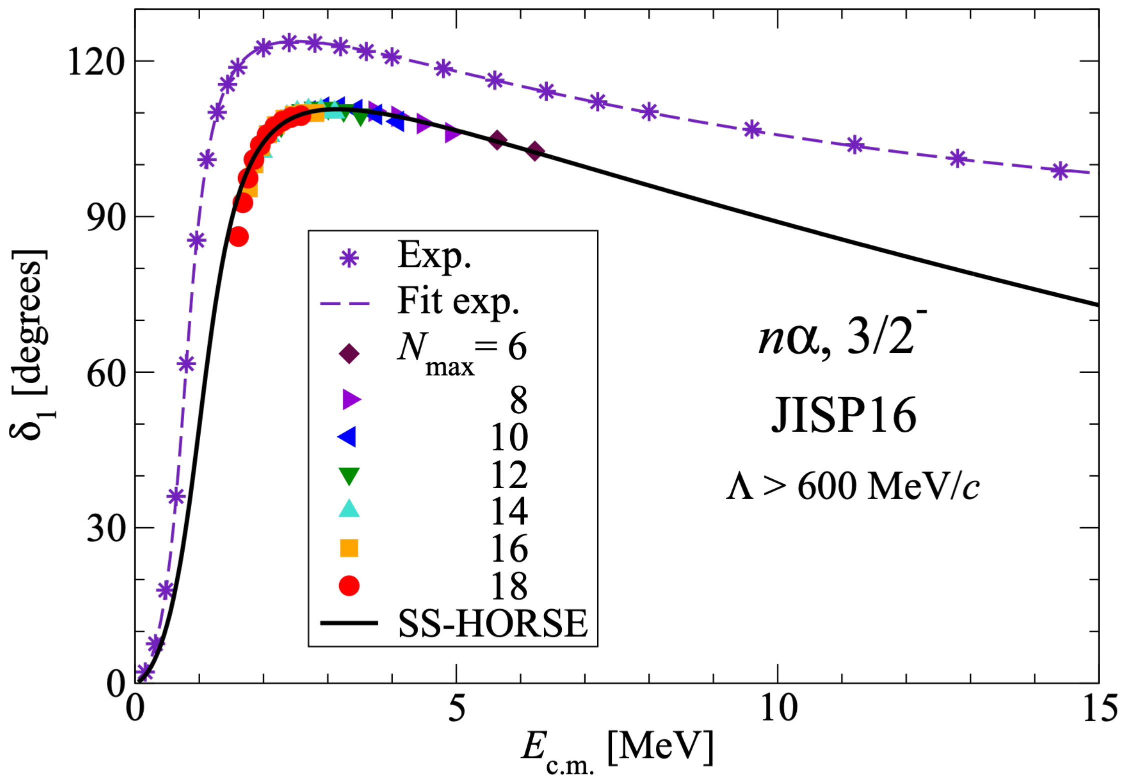
Cf. Shirokov *et al*, PRC **94**, 064320 (2016) ← equivalent to **matching**

- To get discretized scattering states low in energy,
requires large model space

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY

Application of J-matrix to NCSM



N_{max}=6 dim = 3,944
N_{max}=18 dim = 643M

PRC **94**, 064320 (2016), Shirokov, Mazur, Mazur, Vary
"SS-HORSE" a variant of J-matrix

	Standard	Novel
Scattering State basis		Oscillator or other L^2-integrable
Extract phase shift/ S-matrix	Matching	

Technical aside:
truncating the basis
space discretizes the
continuum through a
'boundary condition'….

however:
to get many energies
requires
many basis states

Computing … tr…

- One can … oscillator basis
(“J-matrix … re shell model
Cf. Shirok… valent to **matching**

- Converg… e

The basic idea

We combine two previously used methods in a new approach

- The J-matrix method allows one to represent scattering states in a finite (L^2-integrable) basis, such as harmonic oscillator basis.

- Overlap integrals relate asymptotic behavior (e.g., phase shifts) to integrals over the volume, and can improve convergence.

Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY

	Standard	Novel
Scattering State basis	Coordinate or momentum space	Oscillator or other L^2-integrable
Extract phase shift/ S-matrix	Matching	Overlap/integral

Phys. Rev. C **113**, 024004 (2026)

Flow chart of project

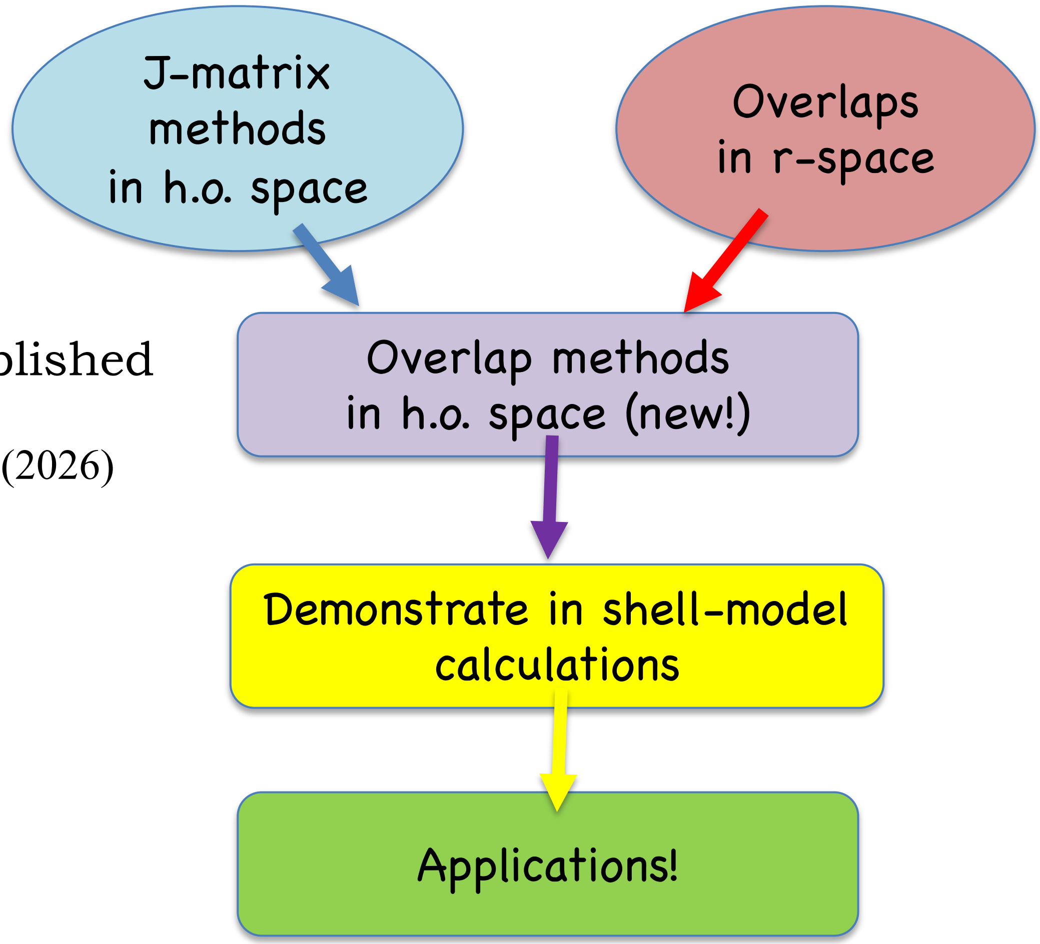
Input concepts:

Foundational paper published

Phys. Rev. C **113**, 024004 (2026)

In progress….

Near future



San Diego State University

We have generalized to finite bases

e.g., harmonic oscillator basis

"scattering overlap relation" = SOR

$$\tan\delta = -\frac{\langle f|V|u\rangle}{\langle g|V|u\rangle + W\,u_o/f_o}$$

Wronskian

correction term (arises from inhomogeneous diff eqn)

SAN DIEGO STATE UNIVERSITY

We have generalized to finite bases

e.g., harmonic oscillator basis

coefficient

"scattering overlap relation" = SOR

$$u(r) = \sum_n u_n \phi_n(r)$$

basis function

$$\tan\delta = -\frac{\langle f|V|u\rangle}{\langle g|V|u\rangle + W\, u_o/f_o}$$

Wronskian

correction term (arises from inhomogeneous diff eqn)

SAN DIEGO STATE UNIVERSITY

We have generalized to finite bases

e.g., harmonic oscillator basis

coefficient

"scattering overlap relation" = SOR

$$u(r) = \sum_n u_n \phi_n(r)$$

basis function

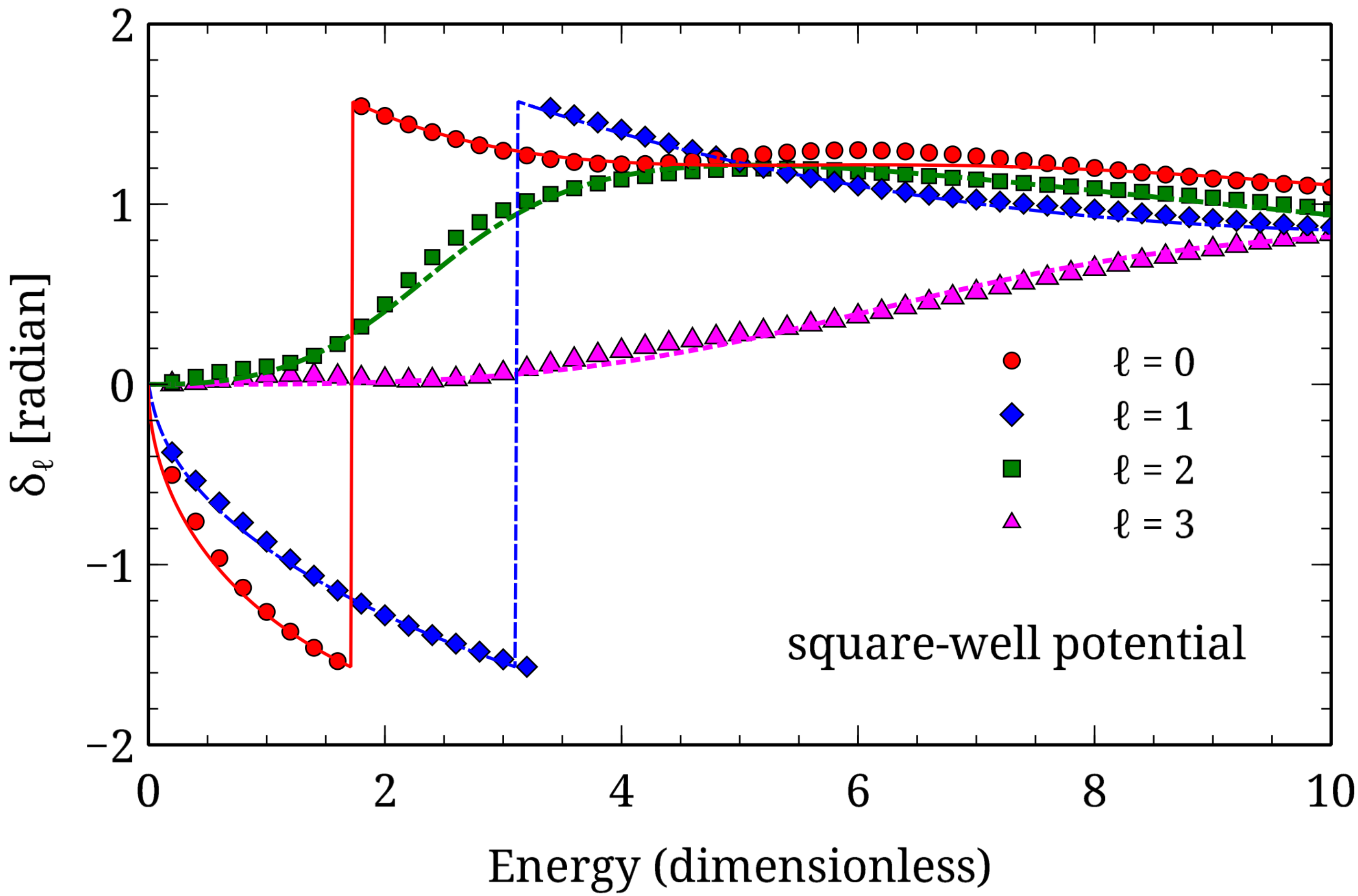
$$\tan\delta = \frac{B}{A} = -\frac{\sum_{n=0}^{N_{\mathrm{pot}}} f_n \sum_{m=0}^{N_{\mathrm{pot}}} V_{n,m} u_m}{\alpha_0 u_0 + \sum_{n=0}^{N_{\mathrm{pot}}} g_n \sum_{m=0}^{N_{\mathrm{pot}}} V_{n,m} u_m}.$$

correction term (arises from inhomogeneous diff eqn)

Scattering in a shell-model basis

San Diego State University

Full scattering solutions generated via Lippmann-Schwinger at any energy



Scattering in a shell-model basis

Full scattering solutions generated
via Lippmann-Schwinger at any energy

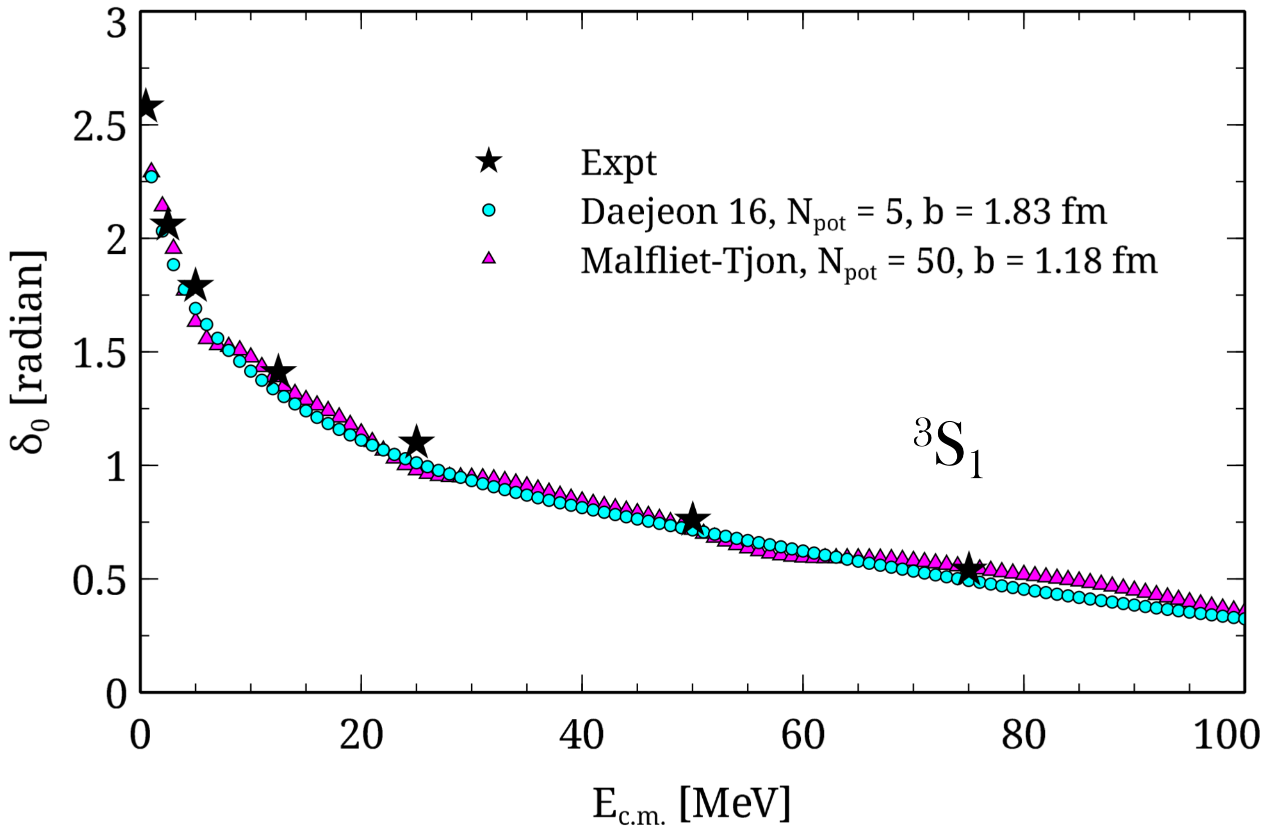
$$|u_{scatt}\rangle = |free\rangle + \frac{1}{E-H} V|free\rangle$$

Full Hamiltonian

Works well in potential scattering
using h.o. basis.

Scattering in a shell-model basis

San Diego State University



San Diego State University

Flow chart of project

Input concepts:

J-matrix methods in h.o. space

Overlaps in r-space

Foundational paper published

Phys. Rev. C **113**, 024004 (2026)

Overlap methods in h.o. space (new!)

In progress….

Demonstrate in shell-model calculations

Near future

Applications!

San Diego State University

Our accomplishments

- Demonstrated SOR works well in harmonic oscillator space
(in fact, better than in coordinate space)

- More rigorous derivation of overlap relations,
including origin of correction term (from inhom. diff. eq.)

- Published initial paper— (after many fights with referees…)

SAN DIEGO STATE UNIVERSITY

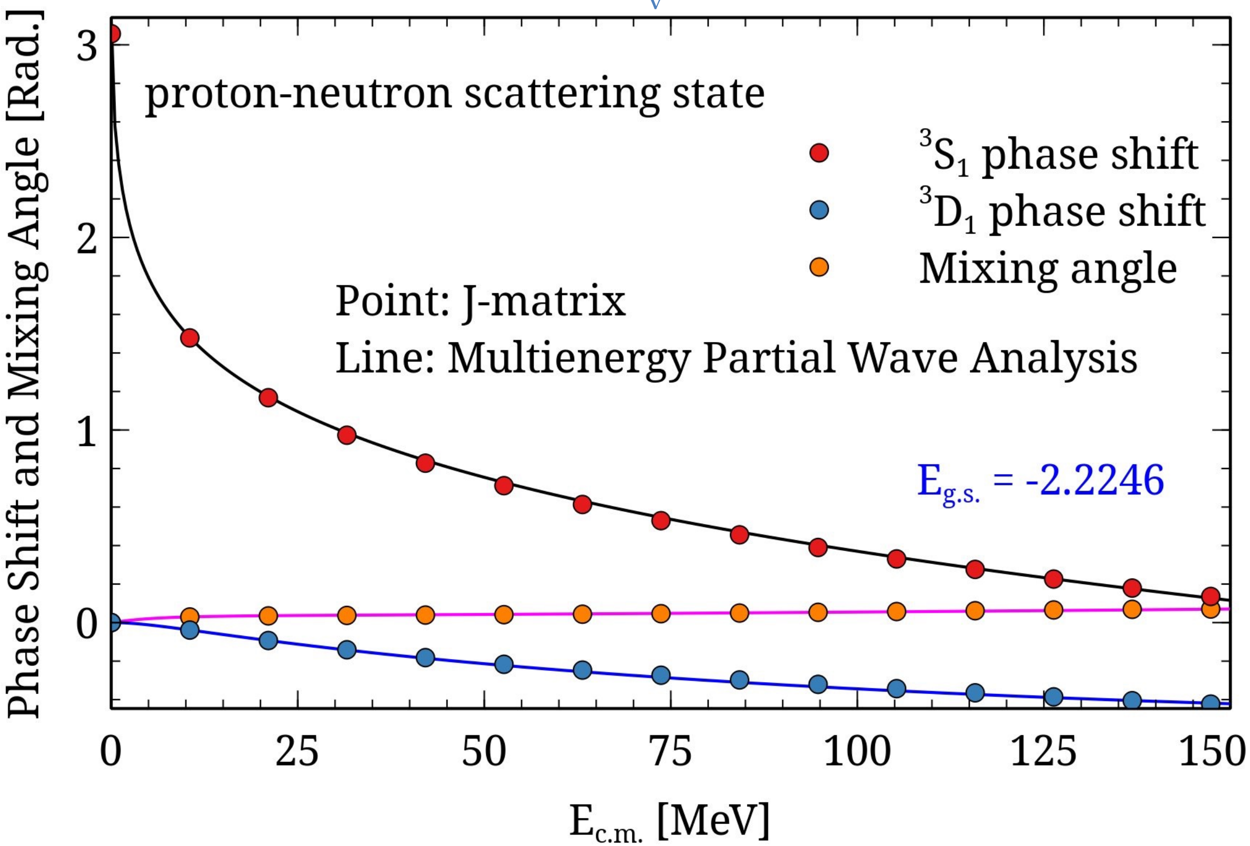
Recent Work

- Extension to coupled-channels S-matrices
- **First implementation in (independent-particle) shell-model**
- (Developed formalism for generalized bases, incl. Coulomb)

SAN DIEGO STATE UNIVERSITY

In progress

- Generalization to coupled-channel S-matrices



Preliminary

Shell-model implementation (ind. particle)

Zeroth step: generate an effective potential from a frozen core in harmonic oscillator basis, similar to mean-field potential (but with exact Pauli exclusion)

SAN DIEGO STATE UNIVERSITY

Shell-model implementation (ind. particle)

Zeroth step: generate an effective potential from a frozen core in harmonic oscillator basis, similar to mean-field potential (but with exact Pauli exclusion)

Let V(ac,bd) = $\langle ac|V|bd\rangle$ be two-body shell-model matrix elements

$$V_{eff}(a,b) = \sum_{c,d} V(ac,bd)\rho(c,d)$$

Shell-model implementation (ind. particle)

Zeroth step: generate an effective potential from a frozen core in harmonic oscillator basis, similar to mean-field potential (but with exact Pauli exclusion)

Let V(ac,bd) = $\langle ac|V|bd\rangle$ be two-body shell-model matrix elements

$$V_{eff}(a,b) = \sum_{c,d} V(ac,bd)\rho(c,d)$$

Now assume a frozen core, ρ(c,d) = δ(c,d), c in core

$$V_{eff}(a,b) = \sum_{c \in \text{core}} V(ac,bc)$$

SAN DIEGO STATE UNIVERSITY

Shell-model implementation (ind. particle)

Z … nic

c … lusion)

I

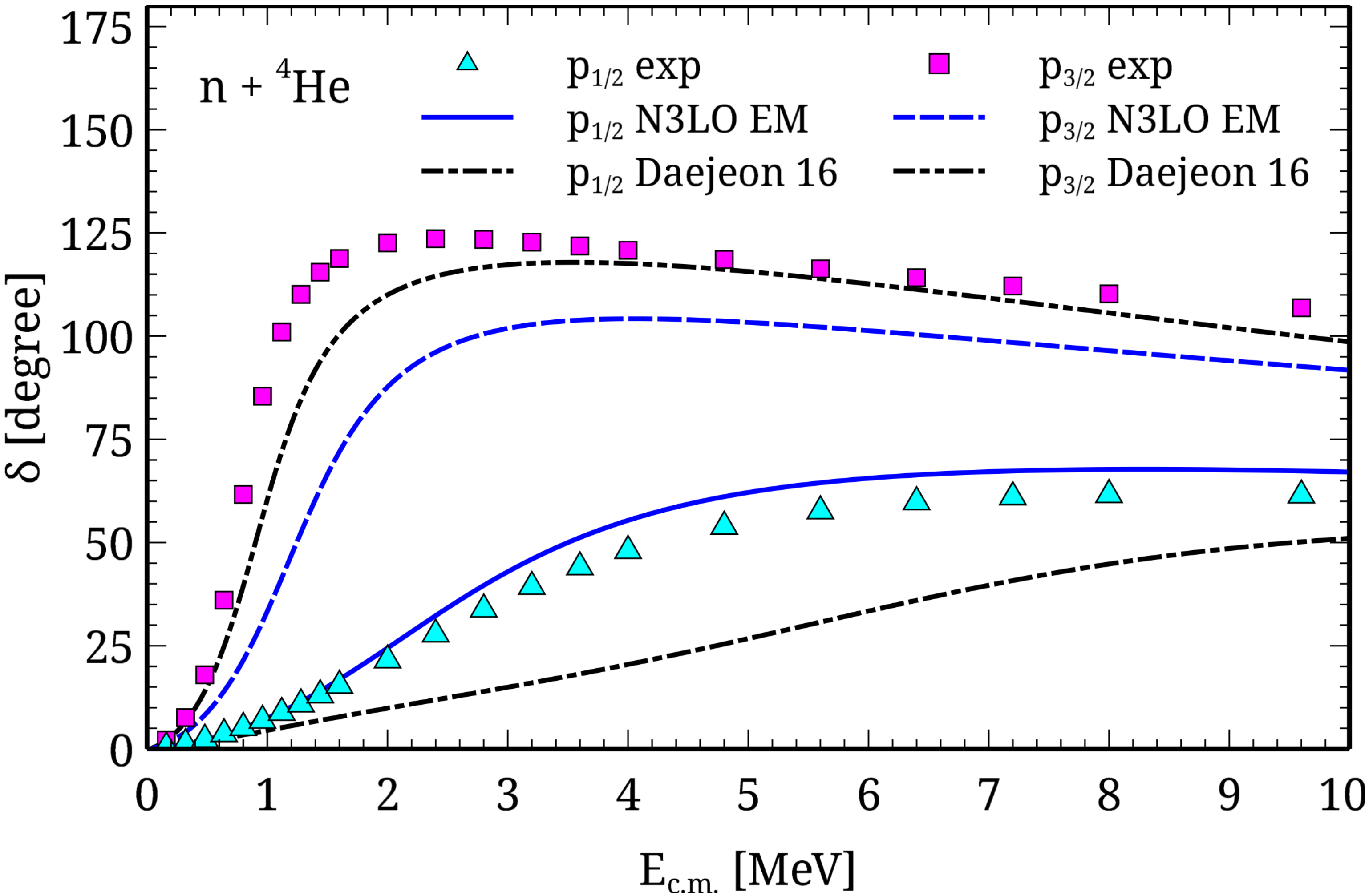
N

This is an effective potential due to the frozen target (^4He, ^{16}O, ^{40}Ca) in a h.o. basis

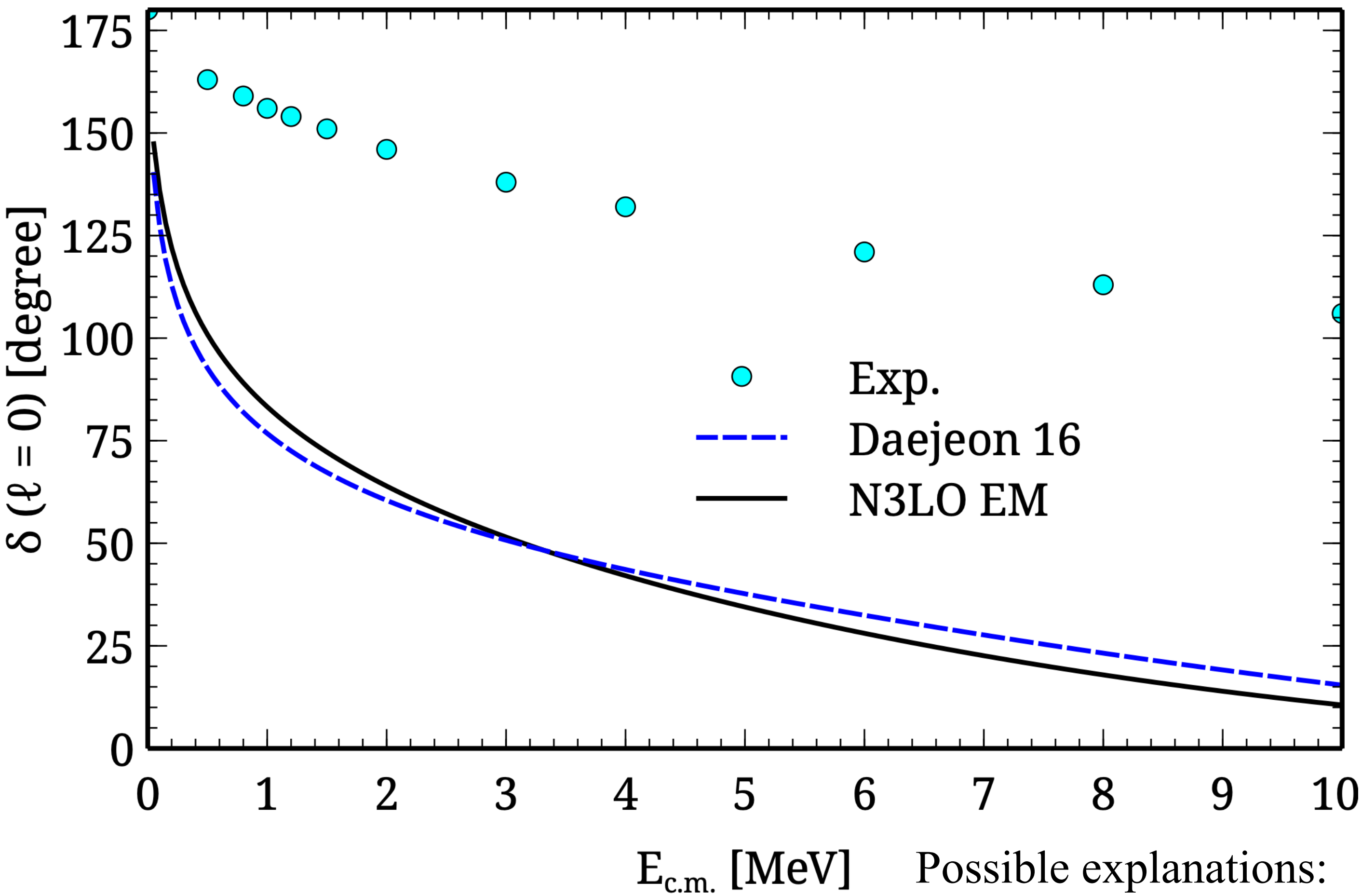
We add in KE matrix elements, find solutions using Lippmann-Schwinger, and apply SOR

$$V_{eff}(a,b) = \sum_{c \in \text{core}} V(ac, bc)$$

Scattering in a shell-model basis



Scattering in a shell-model basis

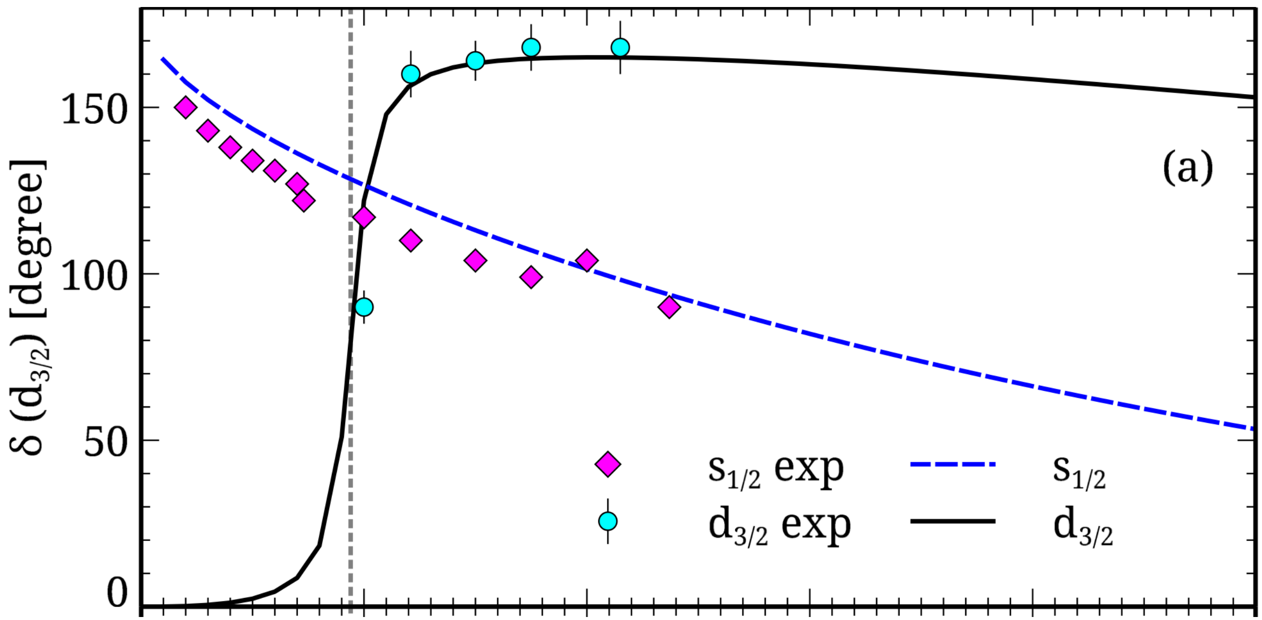


n+^{4}He $s_{1/2}$ phase shift

Possible explanations:
s-wave penetrates deeper-> poor density profile
Center-of-mass?
Not single-particle in character?

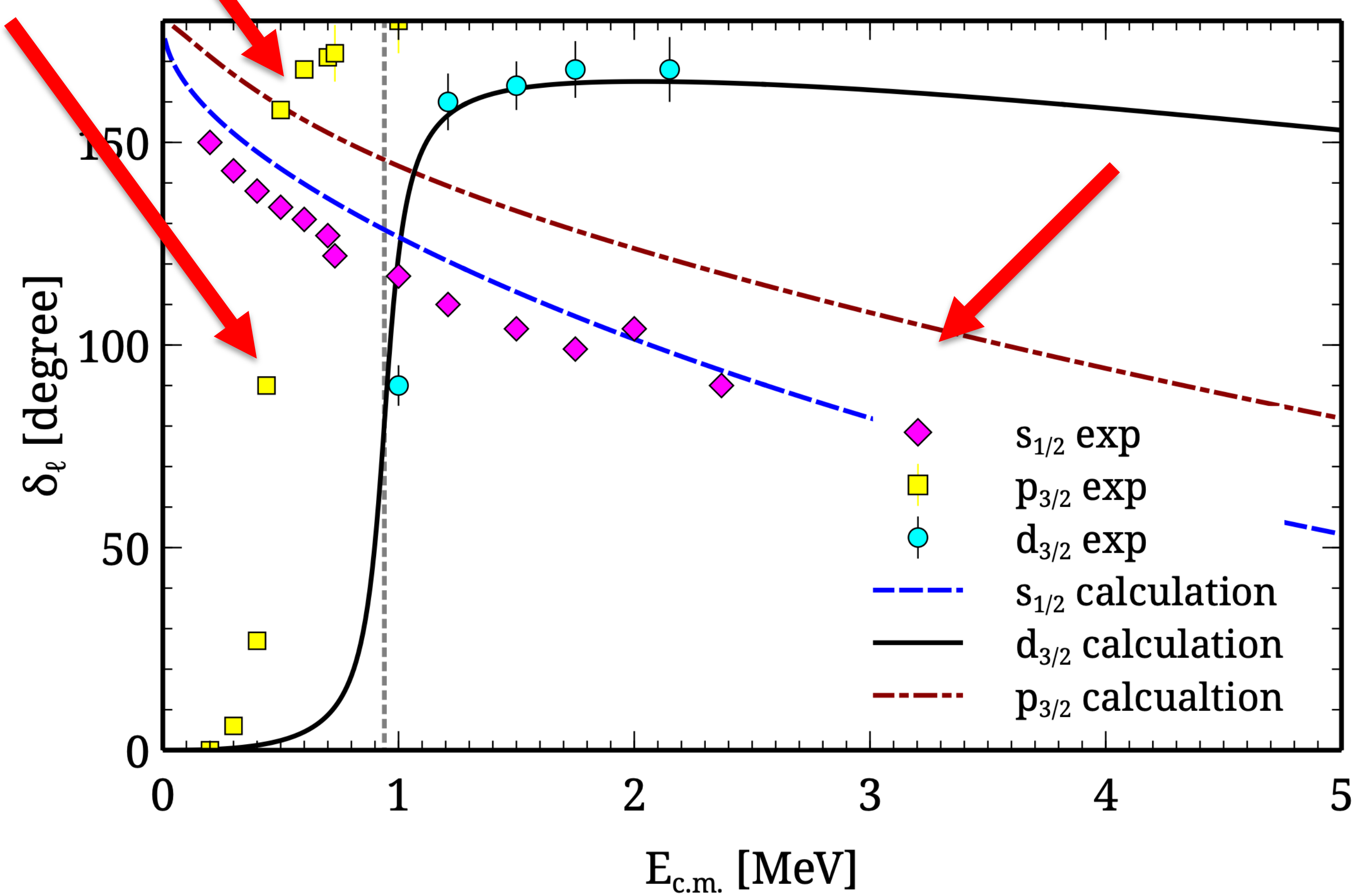
Scattering in a shell-model basis

SAN DIEGO STATE UNIVERSITY



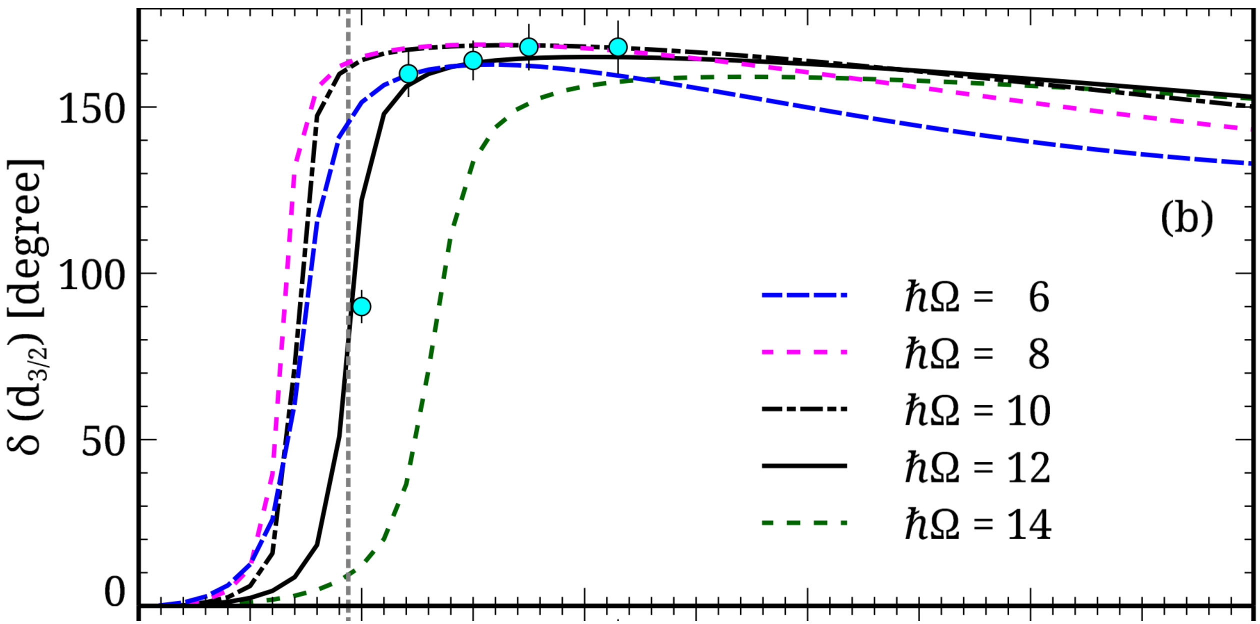
n+^{16}O

n+^{16}O



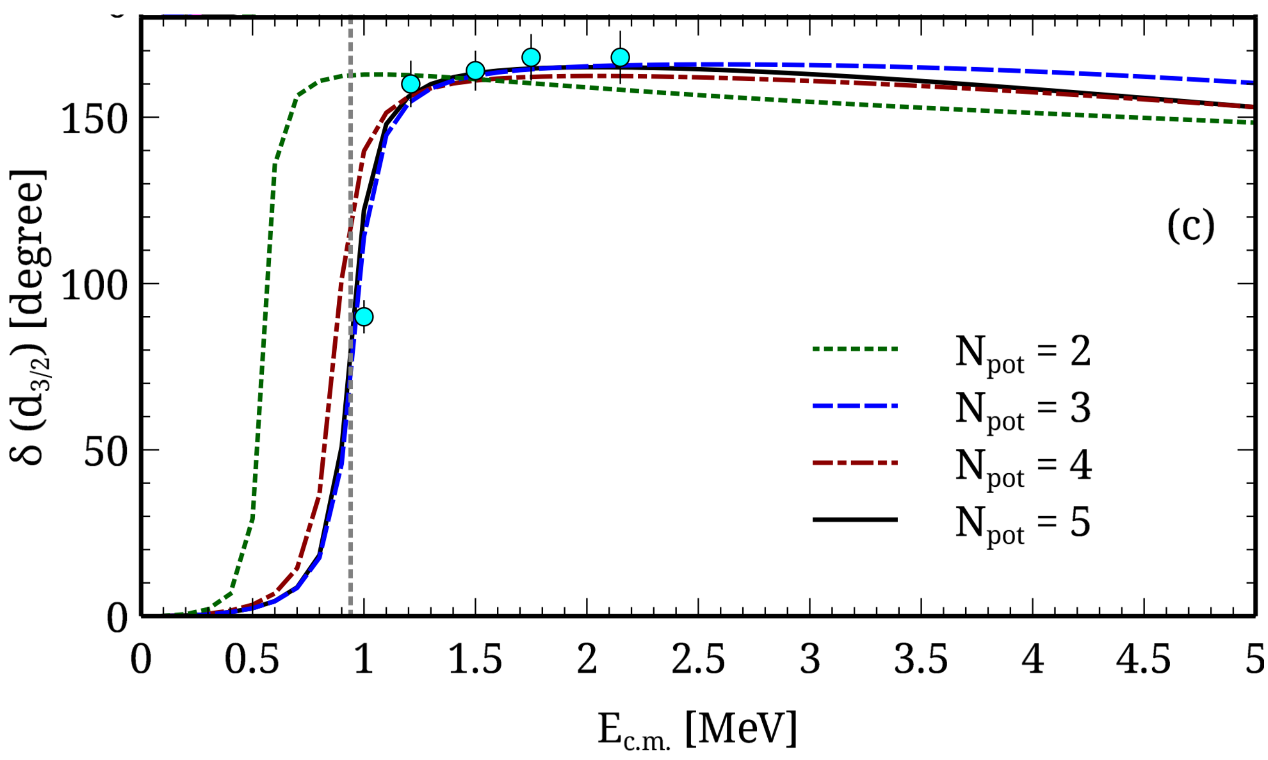
150
100
50
0
0
1
2
3
4
5
δ_ℓ [degree]
E_c.m. [MeV]
s_1/2 exp
p_3/2 exp
d_3/2 exp
s_1/2 calculation
d_3/2 calculation
p_3/2 calcualtion

n+^{16}O



n+^{16}O

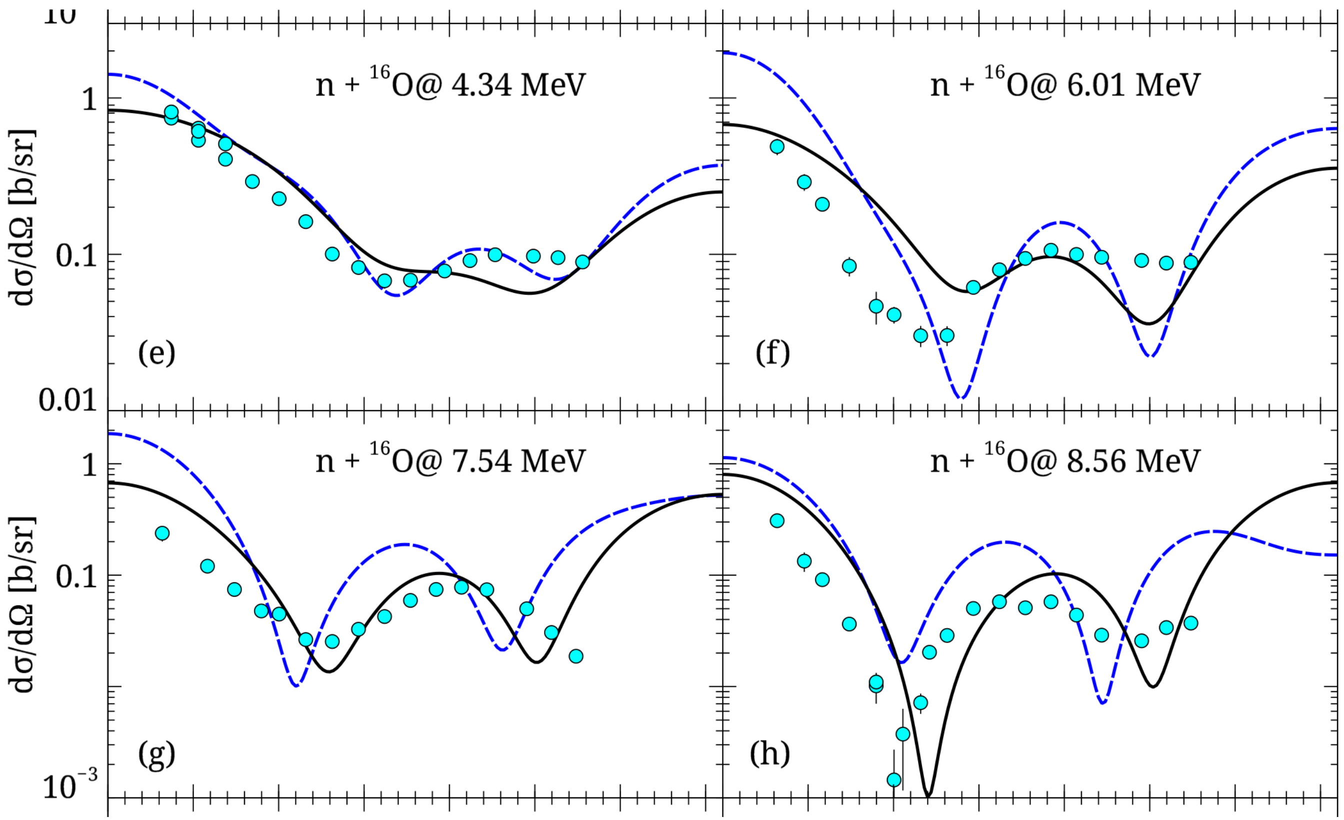
n+^{16}O



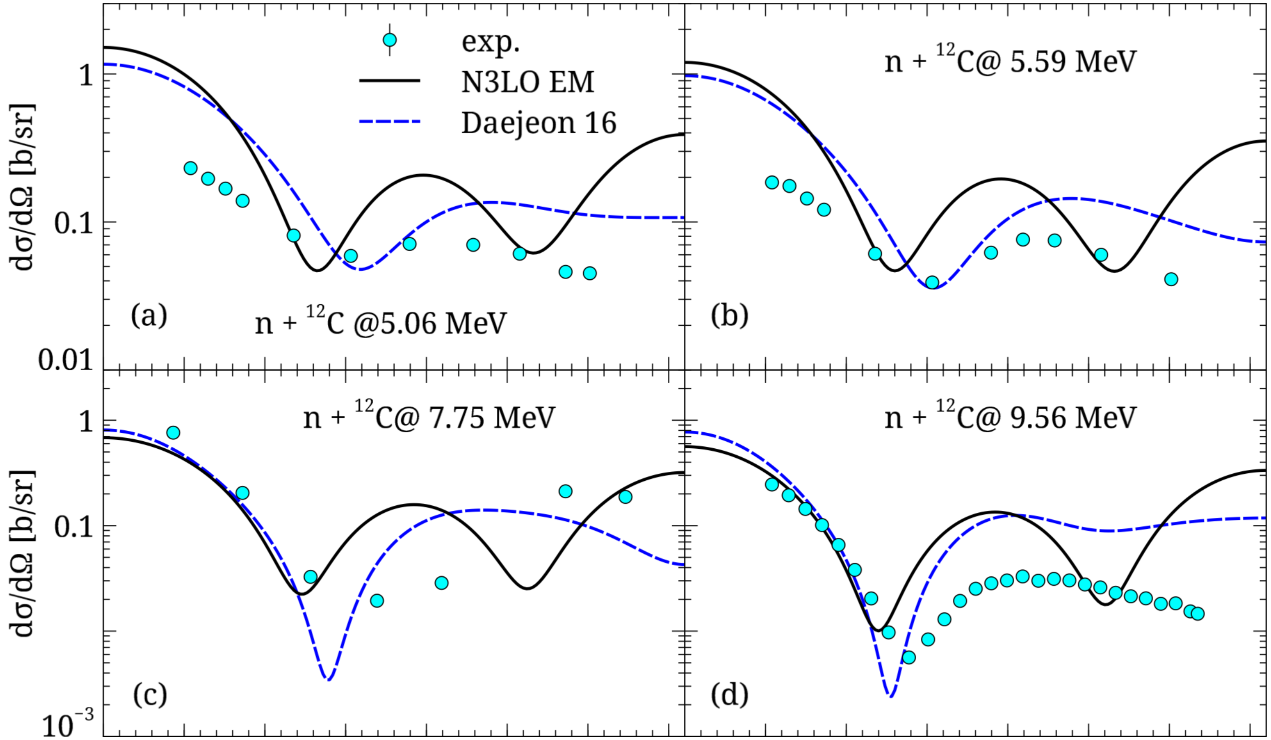
δ (d3/2) [degree]
Ec.m. [MeV]
(c)
Npot = 2
Npot = 3
Npot = 4
Npot = 5
0
50
100
150
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5

n+^{16}O

SAN DIEGO STATE UNIVERSITY

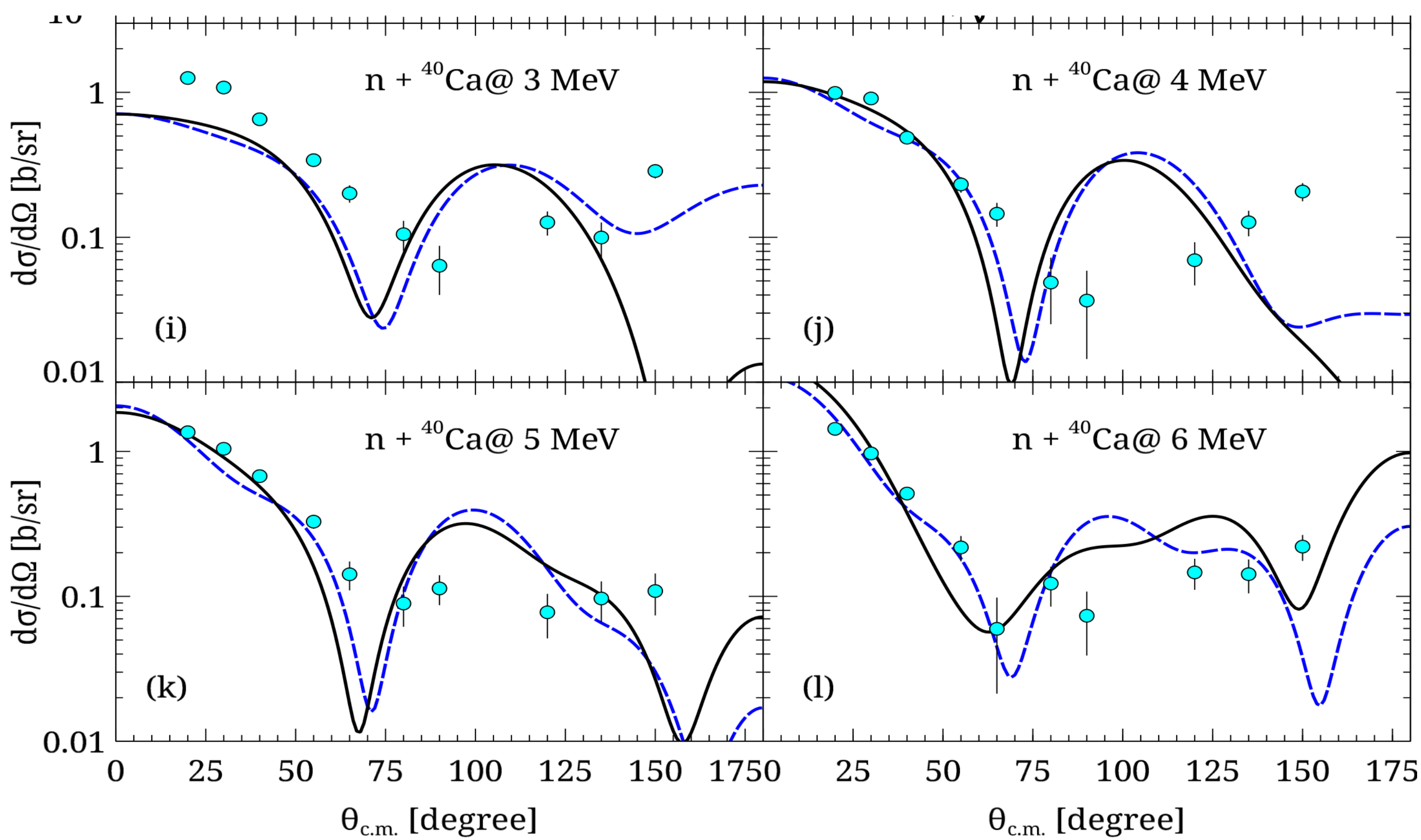


Scattering in a shell-model basis



$n+^{12}C$

n+^{40}Ca



n + 40Ca@ 3 MeV
n + 40Ca@ 4 MeV
n + 40Ca@ 5 MeV
n + 40Ca@ 6 MeV
(i)
(j)
(k)
(l)
dσ/dΩ [b/sr]
θc.m. [degree]

What would a full NCSM calculation look like?

Probably something like the NCSM/RGM or NCSMC formalism, but with SOR pasted in.

$$
\begin{aligned}
&{}_{\mathrm{SD}}\langle \Phi^{J^\pi T}_{\nu' n'} | \hat{P}_{A,A-1} V_{A-2,A-1} | \Phi^{J^\pi T}_{\nu n} \rangle_{\mathrm{SD}} \\
&= \frac{1}{2(A-1)(A-2)} \sum_{jj'K\tau} \sum_{n_a l_a j_a} \sum_{n_b l_b j_b} \sum_{n_c l_c j_c} \sum_{n_d l_d j_d} \sum_{K_a \tau_a K_{cd} \tau_{cd}} \hat{s}\hat{s}'\hat{j}\hat{j}'\hat{K}\hat{\tau}\hat{K}_a\hat{\tau}_a\hat{K}_{cd}\hat{\tau}_{cd}(-1)^{I_1'+j'+J+K+j+j_a+j_c+j_d}(-1)^{T_1+\frac{1}{2}+\tau+T} \\
&\times \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ \ell & J & j \end{Bmatrix} \begin{Bmatrix} I_1' & \frac{1}{2} & s' \\ \ell' & J & j' \end{Bmatrix} \begin{Bmatrix} I_1 & K & I_1' \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} K_a & K_{cd} & K \\ j' & j & j_a \end{Bmatrix} \begin{Bmatrix} T_1 & \tau & T_1' \\ \frac{1}{2} & T & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \tau & \tau_a & \tau_{cd} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \sqrt{1+\delta_{(n_a l_a j_a),(n'\ell' j')}}\sqrt{1+\delta_{(n_c l_c j_c),(n_d l_d j_d)}} \\
&\times \left\langle \left(n'\ell' j' \frac{1}{2}\right)\left(n_a l_a j_a \frac{1}{2}\right) K_{cd}\tau_{cd} \middle| V \middle| \left(n_d l_d j_d \frac{1}{2}\right)\left(n_c l_c j_c \frac{1}{2}\right) K_{cd}\tau_{cd} \right\rangle \\
&\times {}_{\mathrm{SD}}\langle A-1\, \alpha_1' I_1' T_1' ||| \left(\left(a^\dagger_{n\ell j \frac{1}{2}} a^\dagger_{n_a l_a j_a \frac{1}{2}}\right)^{(K_a \tau_a)} \left(\tilde{a}_{n_c l_c j_c \frac{1}{2}} \tilde{a}_{n_d l_d j_d \frac{1}{2}}\right)^{(K_{cd}\tau_{cd})}\right)^{(K\tau)} ||| A-1\, \alpha_1 I_1 T_1 \rangle_{\mathrm{SD}}. \qquad (52)
\end{aligned}
$$

SAN DIEGO STATE UNIVERSITY

Next steps

- Implement in NCSM/RGM/C-like formalism
- More general bases, and Coulomb scattering (formalism done)
- Asymptotic normalization coefficients (formalism in progress)

\+ extension to reactions

San Diego State University

Next steps

- Implement in NCSM/RGM/C-like formalism
- More general bases, and Coulomb scattering (formalism done)
- Asymptotic normalization coefficients (formalism in progress)

+ extension to reactions

SAN DIEGO STATE UNIVERSITY

Next steps

- Asymptotic normalization coefficients (formalism in progress)

\+ extension to reactions

See Nollett and Wiringa, Phys. Rev. C **83**, 041001(R) (2011)

$$C = -\frac{1}{2\kappa}\left(u'(0) + \frac{2\mu}{\hbar^2}\int_0^R e^{\kappa r}\,V(r)\,u(r)\,dr\right),$$

SAN DIEGO STATE UNIVERSITY

Next steps

- Asymptotic normalization coefficients (formalism in progress)

+ extension to reactions

See Nollett and Wiringa, Phys. Rev. C **83**, 041001(R) (2011)

$$C = -\frac{1}{2\kappa}\left(u'(0) + \frac{2\mu}{\hbar^2}\int_0^R e^{\kappa r}\, V(r)\, u(r)\, dr\right),$$

u(r) goes like exp(-κ r)

This requires V(r) to fall off fast enough, which it might not in h.o. space

SAN DIEGO STATE UNIVERSITY

Summary

Previous work on J-matrix methods (Heller 1974, Shirokov 2016): one can recast scattering in finite bases e.g. h.o. states

Other work (Kievsky, Nollett, etc) have use integrals/overlaps to extract phase shifts/S-matrices, often for better accuracy

We have successfully combined these in potential scattering. Often we get good results in remarkably small dimensions!

This lays the ground work for embedding in full shell-model (or other many-body) calculations

San Diego State University

What I'm hoping for:

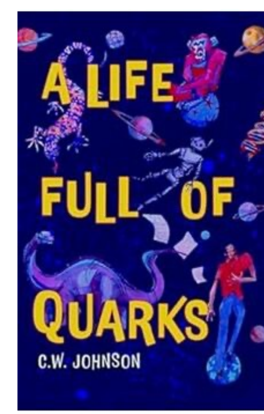
Collaborators/partners interested in further development/applications:

- Apply to shell-model / other many-body methods
- Apply ANCs to reactions

Alternate way to solve coupled channels

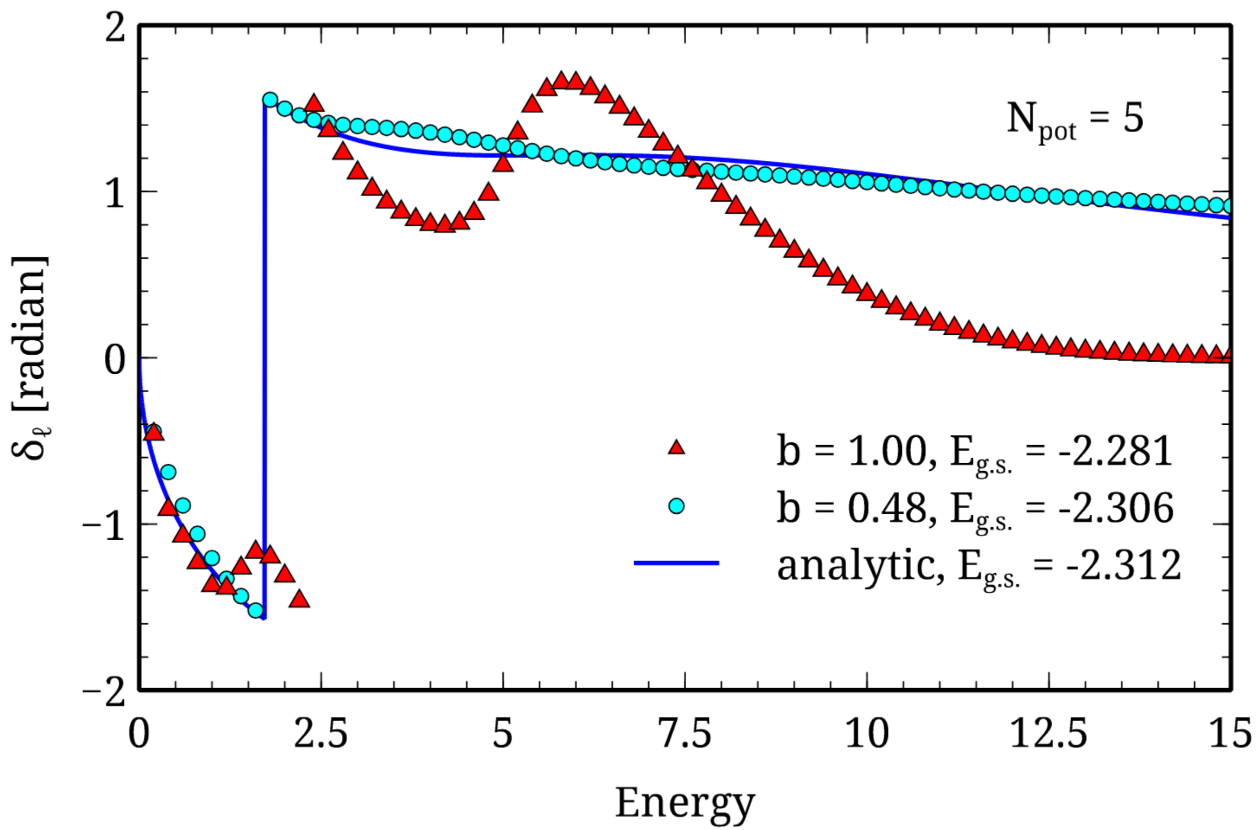
Also:

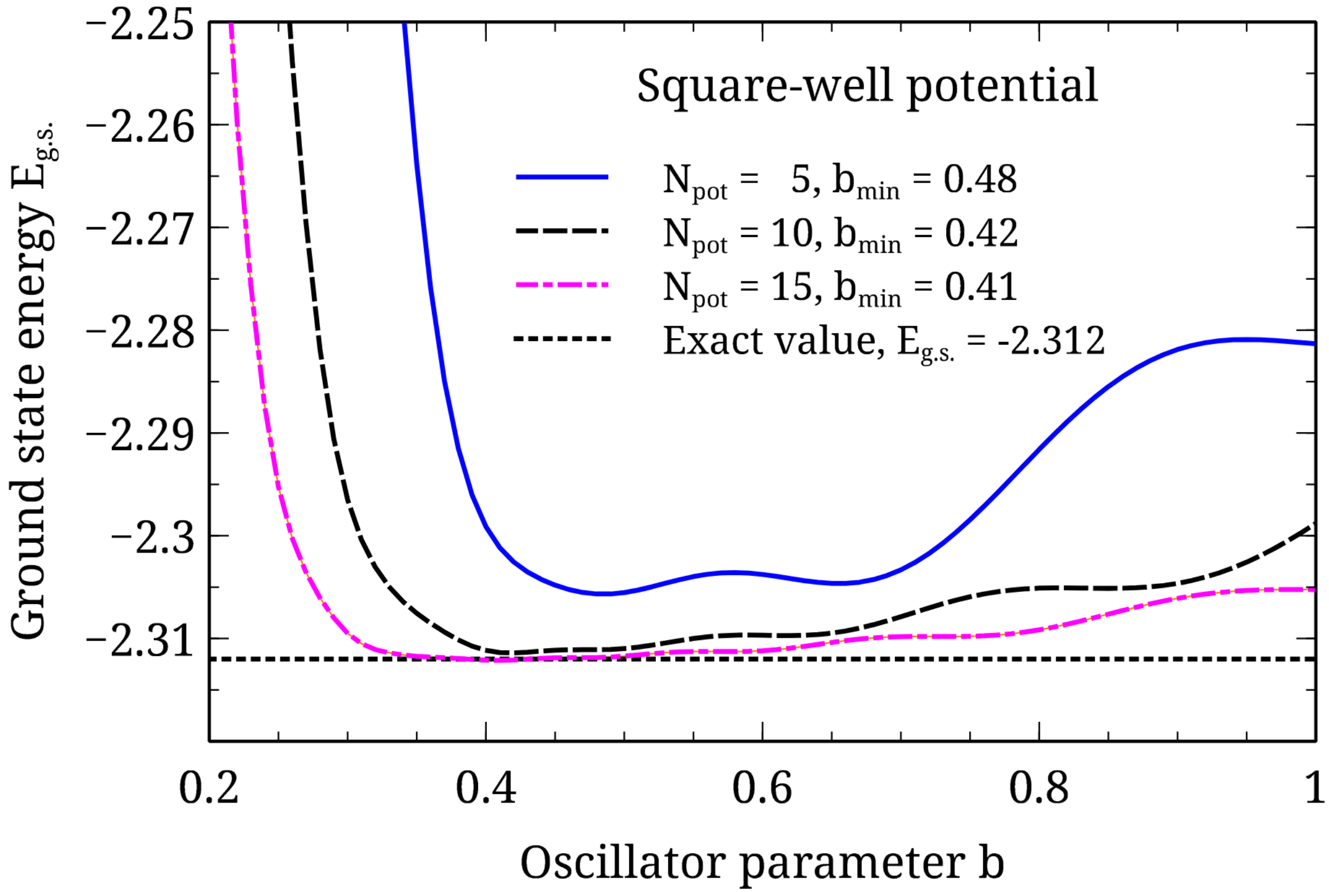
- Extend to Faddeev?



Extra slides

For small dimensions, the quality of the phase shifts is best when `ground state' has minimum energy




Square-well potential
N_{pot} = 5, b_{min} = 0.48
N_{pot} = 10, b_{min} = 0.42
N_{pot} = 15, b_{min} = 0.41
Exact value, $E_{g.s.}$ = -2.312
Ground state energy $E_{g.s.}$
Oscillator parameter b
−2.25
−2.26
−2.27
−2.28
−2.29
−2.3
−2.31
0.2
0.4
0.6
0.8
1

SAN DIEGO STATE UNIVERSITY

Some notes on derivation of SOR in coordinate space

$$\int_0^\infty \left(u_{\rm free} \frac{d^2 u}{dr^2} - u \frac{d^2 u_{\rm free}}{dr^2} \right) dr = \int_0^\infty u_{\rm free}(r) \mathcal{V}(r) u(r)\, dr$$
$$\equiv \langle u_{\rm free} | \mathcal{V} | u \rangle.$$

$$\left(u_{\rm free} \frac{du}{dr} - u \frac{du_{\rm free}}{dr} \right) \Big|_{r=0}^{r\to\infty} = \langle u_{\rm free} | \mathcal{V} | u \rangle.$$

Here, $u_{\rm free}$ is regular (f) or irregular (g) function.

r = infinity yields asymptotic (phase shift), r = 0 yields inhomogeneity

Representation of free functions in finite basis

SAN DIEGO STATE UNIVERSITY

$$f(r) = \sum_{n=0}^{\infty} f_n \phi_n(r)$$

$$\tilde{g}(r) = \sum_{n=0}^{\infty} g_n \phi_n(r) \qquad \lim_{r\to\infty} \tilde{g}(r) \to g(r).$$

Representation of free functions in finite basis

SAN DIEGO STATE UNIVERSITY

$$\tilde{g}(r) = \sum_{n=0}^{\infty} g_n \phi_n(r) \qquad\qquad \lim_{r\to\infty} \tilde{g}(r) \to g(r).$$

$$(\hat{T} - E)\tilde{g}(r) = \alpha_0 \phi_0(r).$$

$$G(r, r') = \frac{g(r_>) f(r_<)}{W(f, g)}$$

$$\begin{aligned} \tilde{g}(r) &= \int_0^\infty G(r, r')\, \alpha_0 \phi_0(r')\, dr' \\ &= \frac{\alpha_0}{W} \left(g(r) \int_0^r f(r') \phi_0(r')\, dr' + f(r) \int_r^\infty g(r') \phi_0(r')\, dr' \right). \end{aligned}$$