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Scattering in a shell-model basis

Calvin W. Johnson

with Minh-Loc Bui and Kenneth M. Nollett

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

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ECT* "Nuclear theory for astrophysics" May 19, 2026

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The team:



Minh-Loc Bui, Postdoc



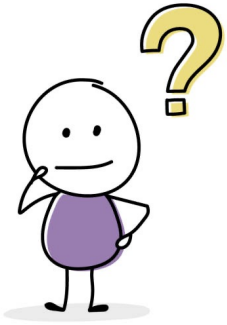


Kenneth M. Nollett





Calvin W. Johnson



Origin Story

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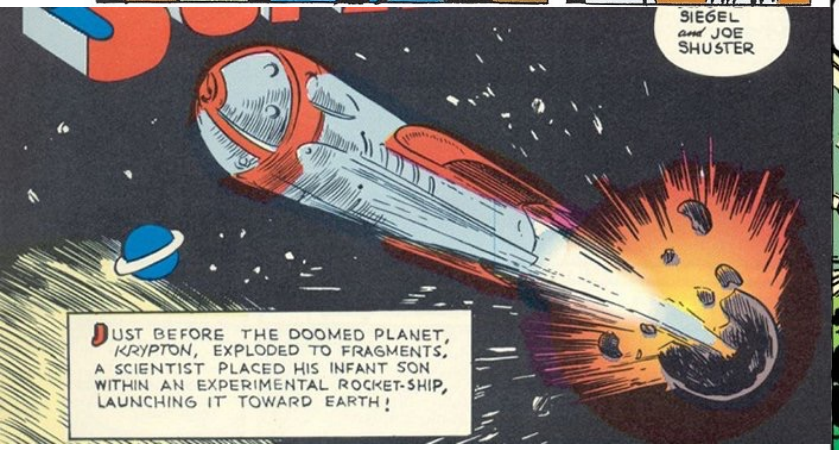





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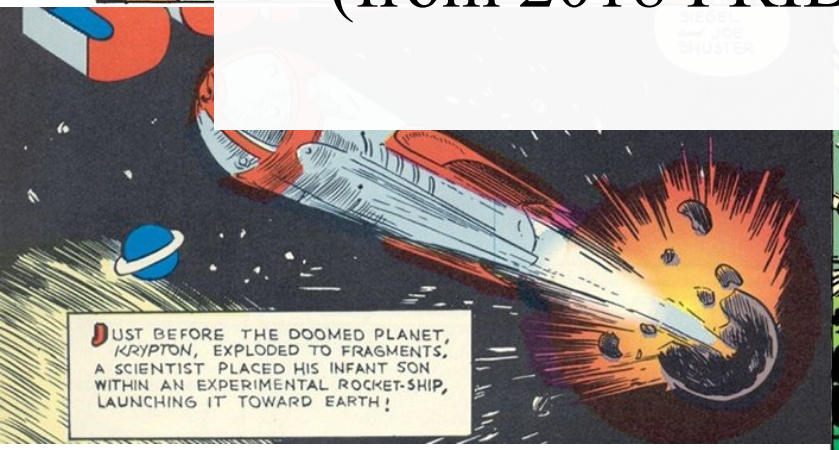
Origin Story



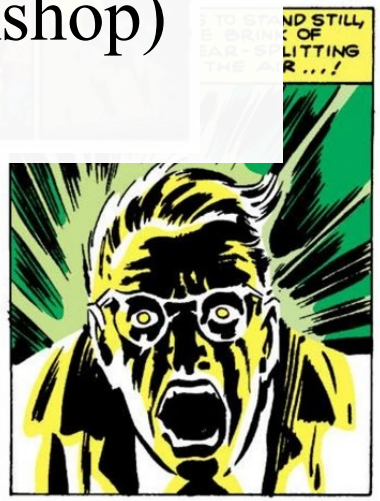


"White Paper: From bound states to the continuum," CWJ, K.Launey, *et al*, J. Phys. G. **47** 123001 (2020) (from 2018 FRIB Theory alliance workshop)











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The goal of the project

To develop and improve scattering and reaction methods;



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The goal of the project

To develop and improve scattering and reaction methods;

(NB: the bulk of this talk is about scattering, looking forward to **direct reactions**.
At the end, I'll talk very briefly about an approach to **statistical reactions** in the shell model)

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The goal of the project

To develop and improve scattering and reaction methods;

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



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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)



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A few words about….

Configuration-interaction shell model

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

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

$$\left|\Psi\right\rangle = \sum_{\alpha} c_{\alpha}\left|\alpha\right\rangle$$

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

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



A few words about….

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

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

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



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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

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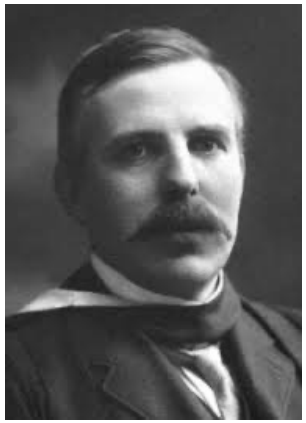

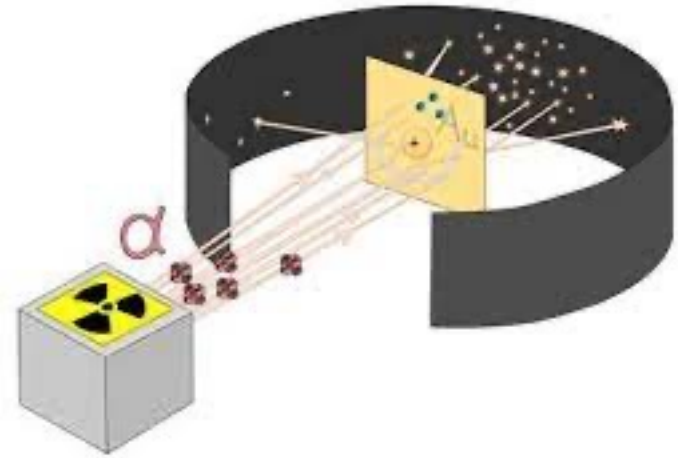

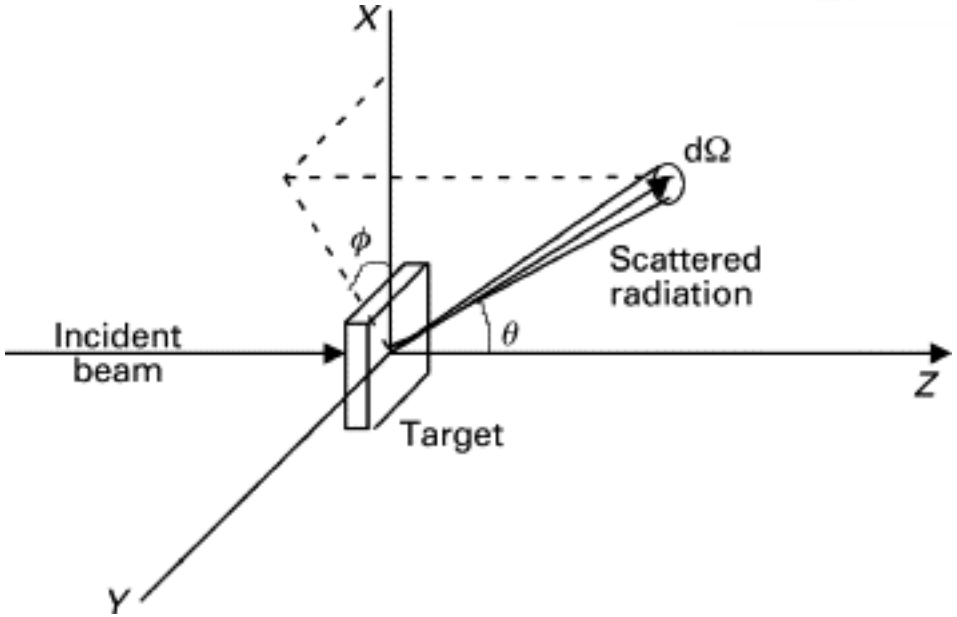

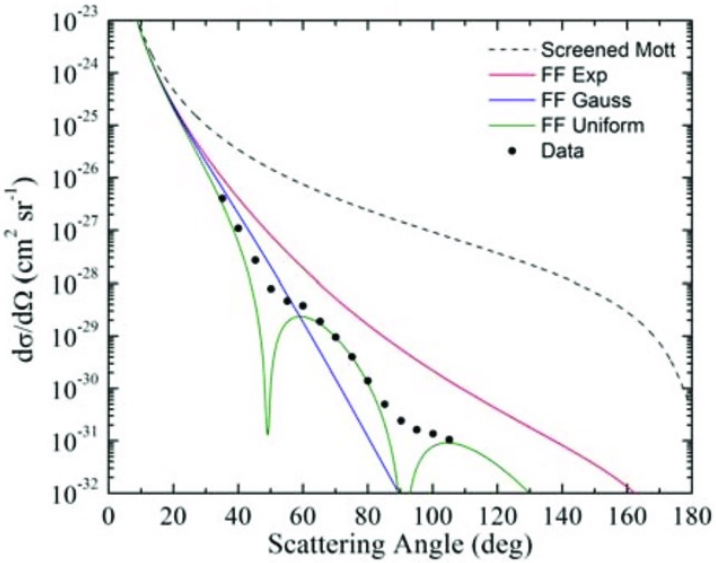

Scattering in a shell-model basis

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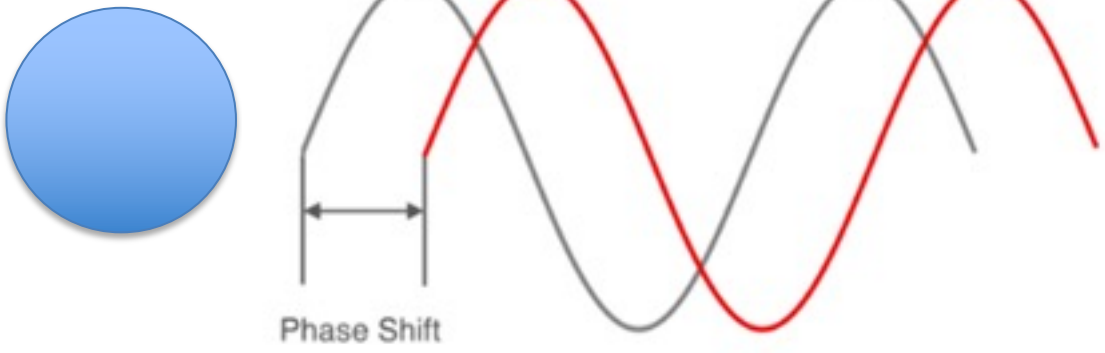

Potential →
Phase shift

Scattering in a shell-model basis

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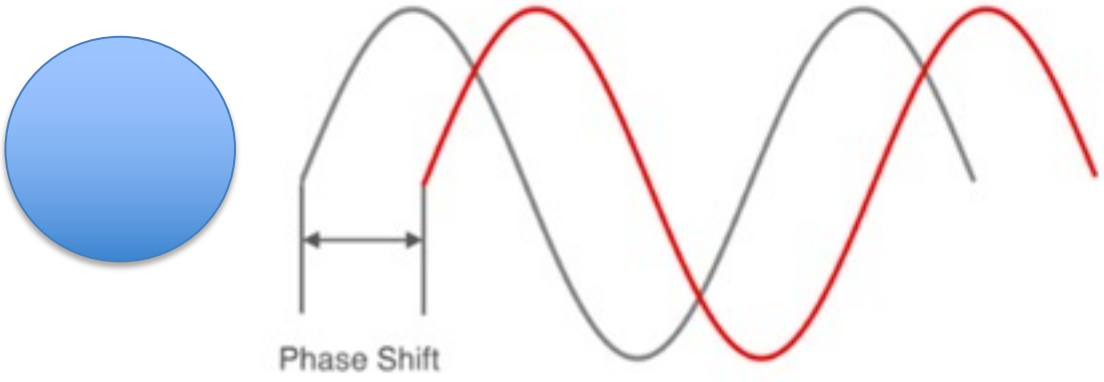
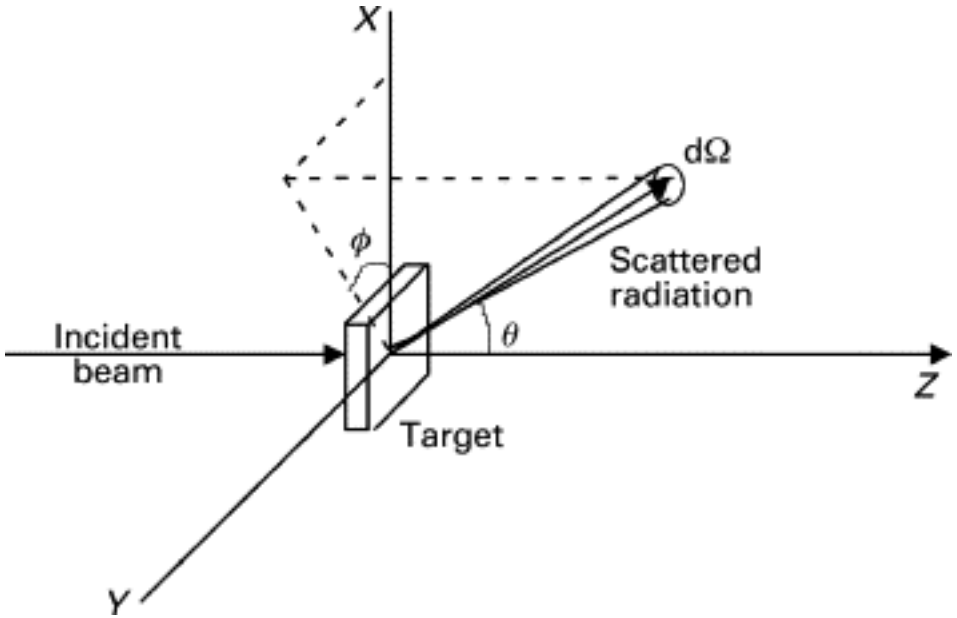
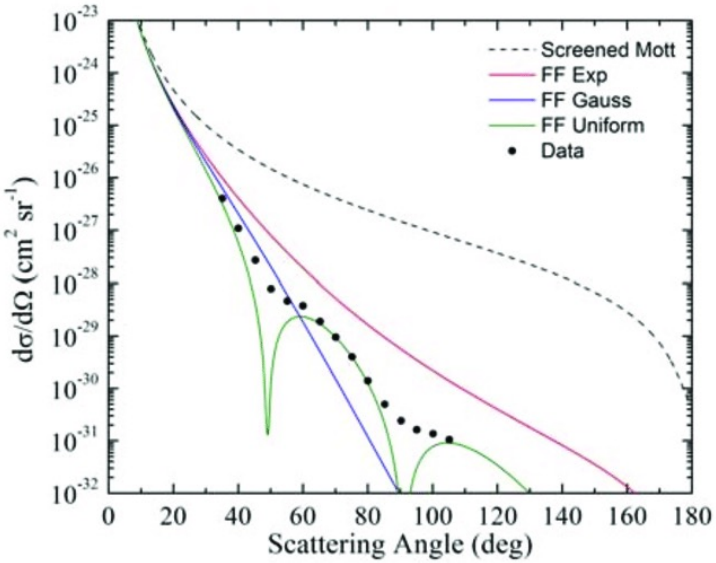


Potential →
Phase shift →
Interference →
Scattering cross-section





Scattering in a shell-model basis

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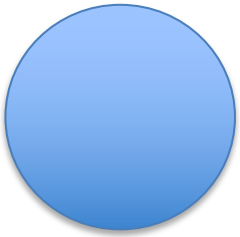
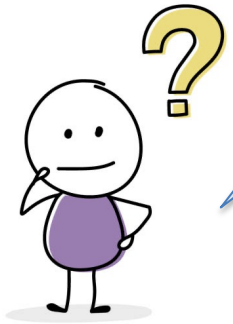
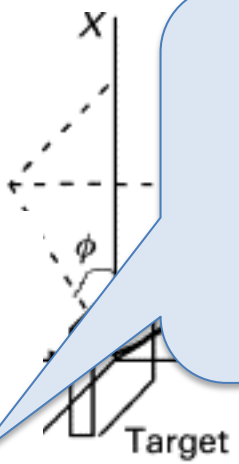


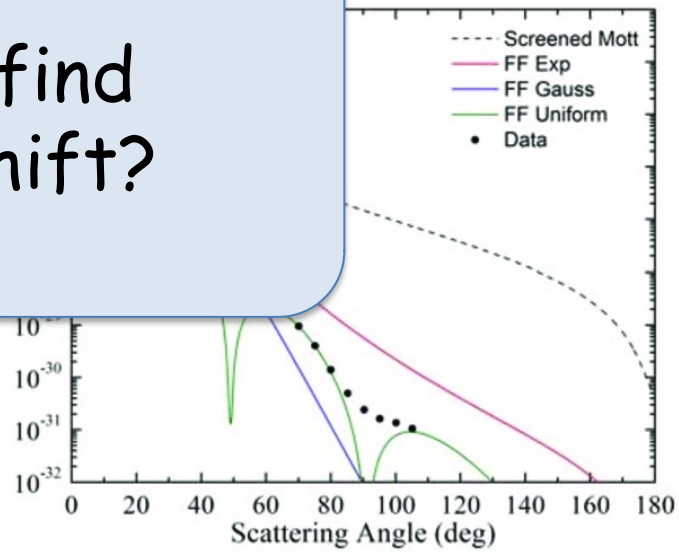


Potential →
Phase shift →
Interference →
Scattering cross-section

How do we find the phase shift?







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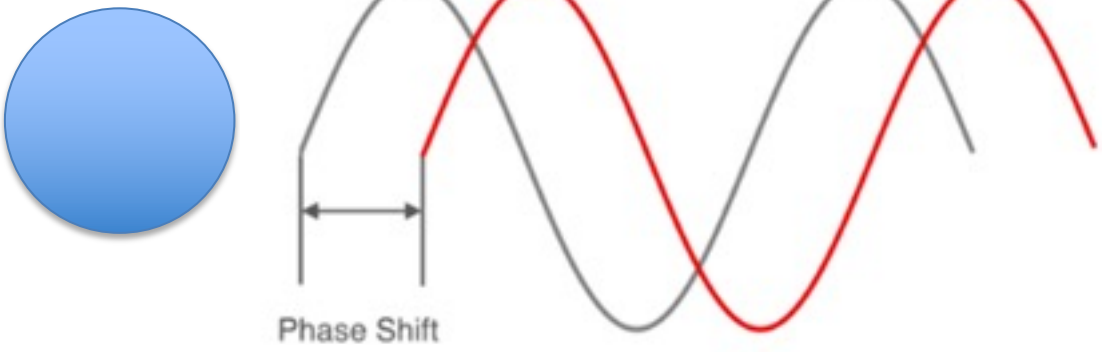
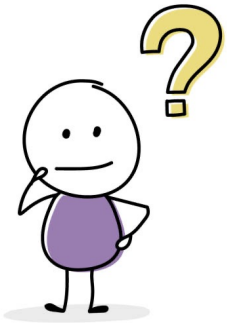
There are **two steps** to computing the phase shift/S-matrix







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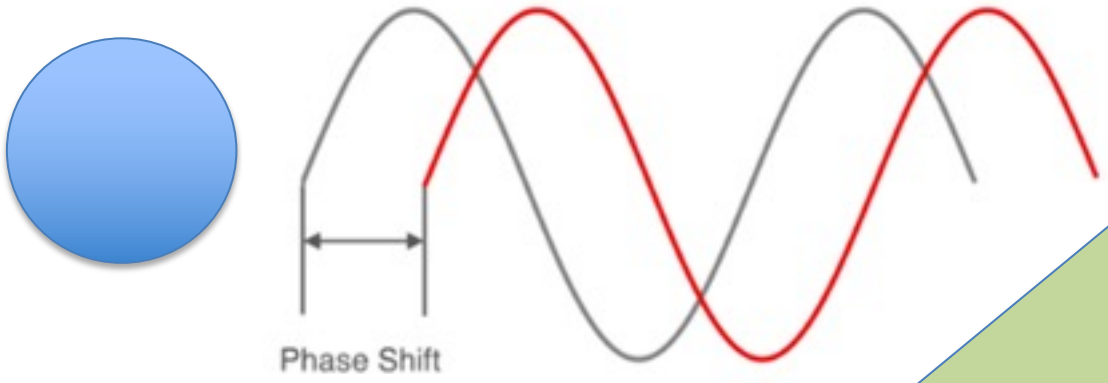
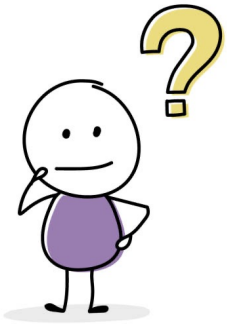


First, generate the scattered state



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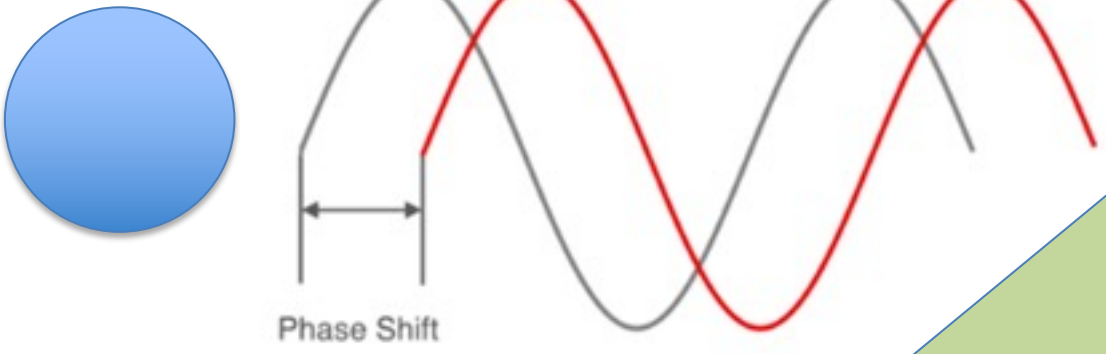
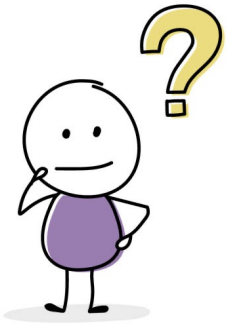
There are **two steps** to computing the phase shift/S-matrix







First, generate the scattered state

Second, extract phase shift/S-matrix

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Standard

Scattering State basis

Coordinate or momentum space



Extract phase shift/ S-matrix

Matching

Scattering in a shell-model basis

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

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One can also swap methods



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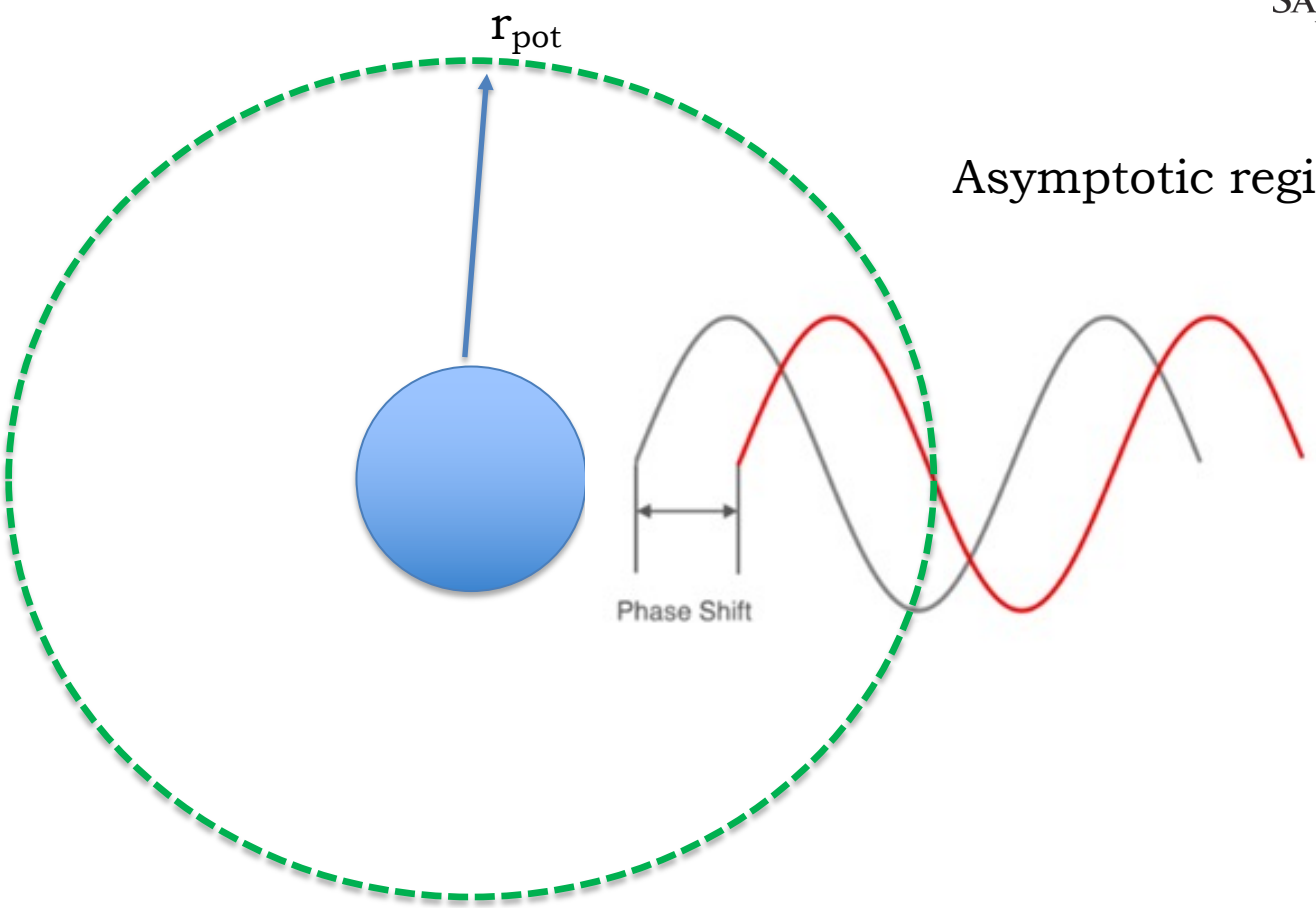

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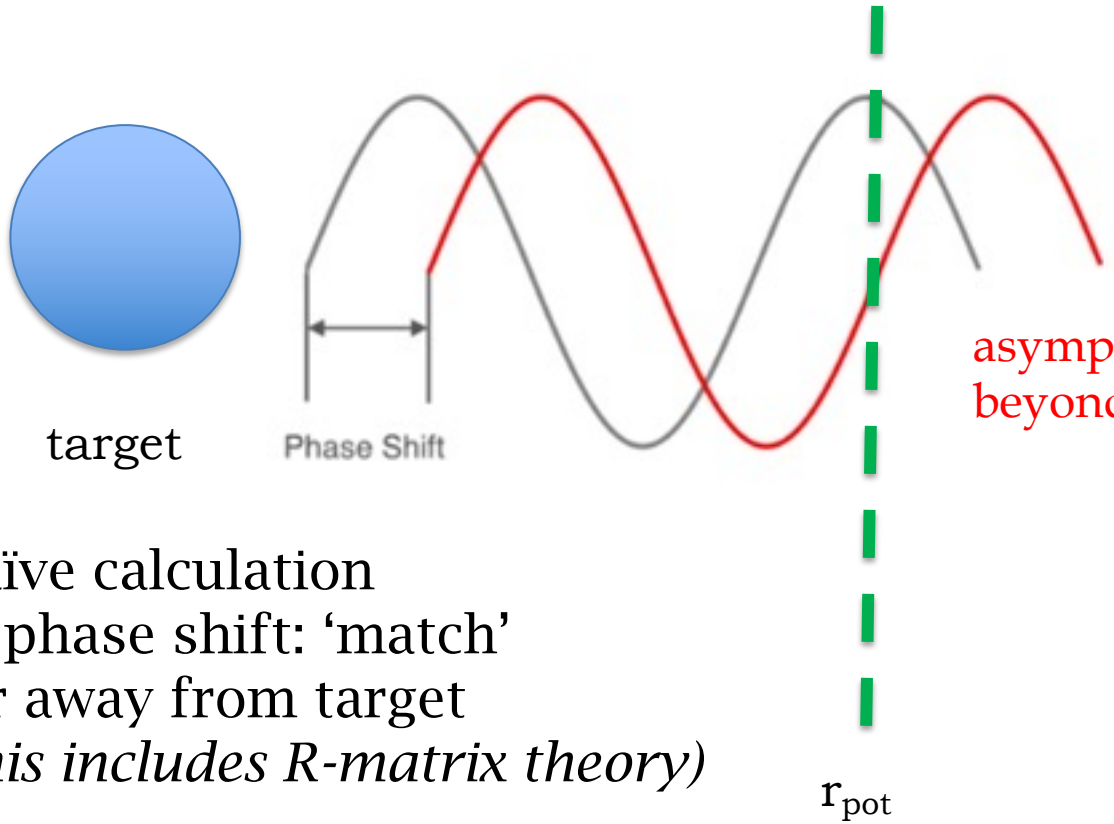
Matching

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)*

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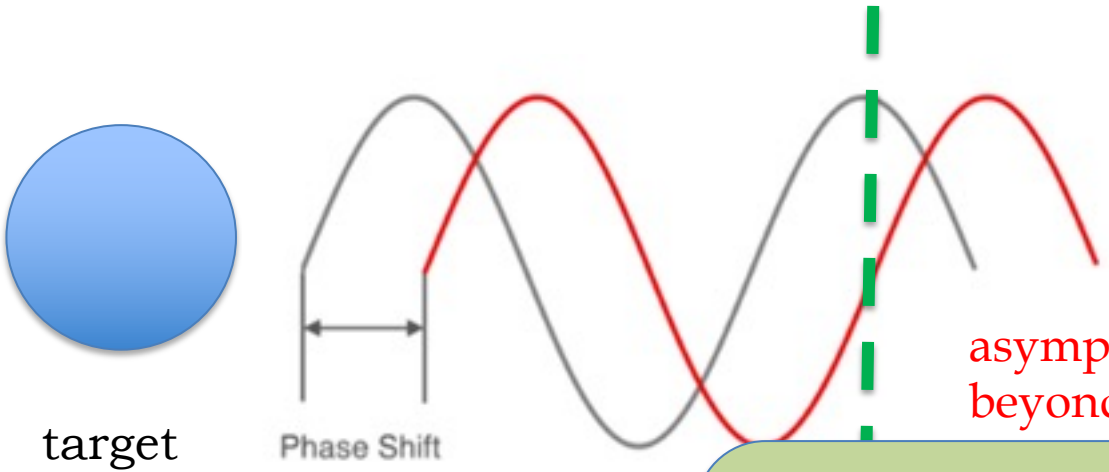
Matching

Potential →
Phase shift →



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



Scattering in a shell-model basis

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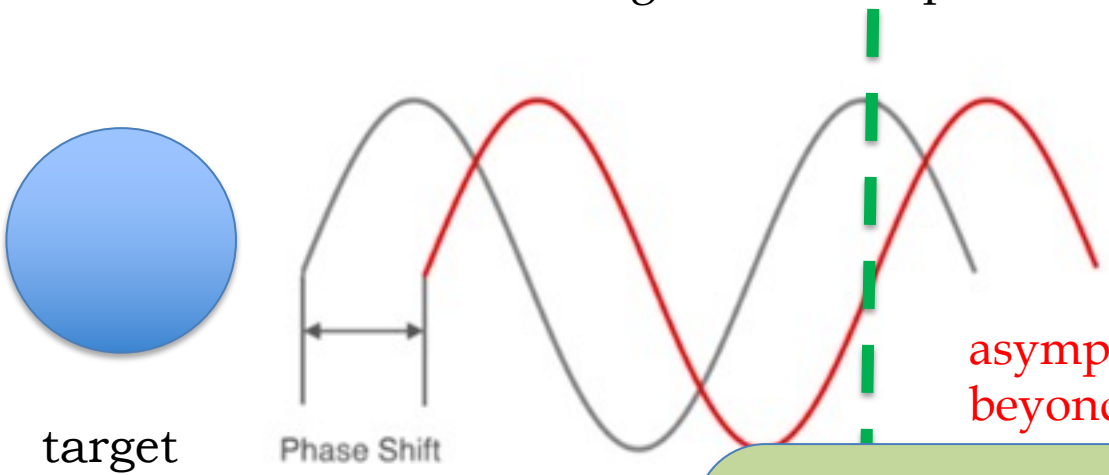
$$u_{asymp}(r) = f(r) + \sin\delta \; g(r)$$

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



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Scattering in a shell-model basis



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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



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

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(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

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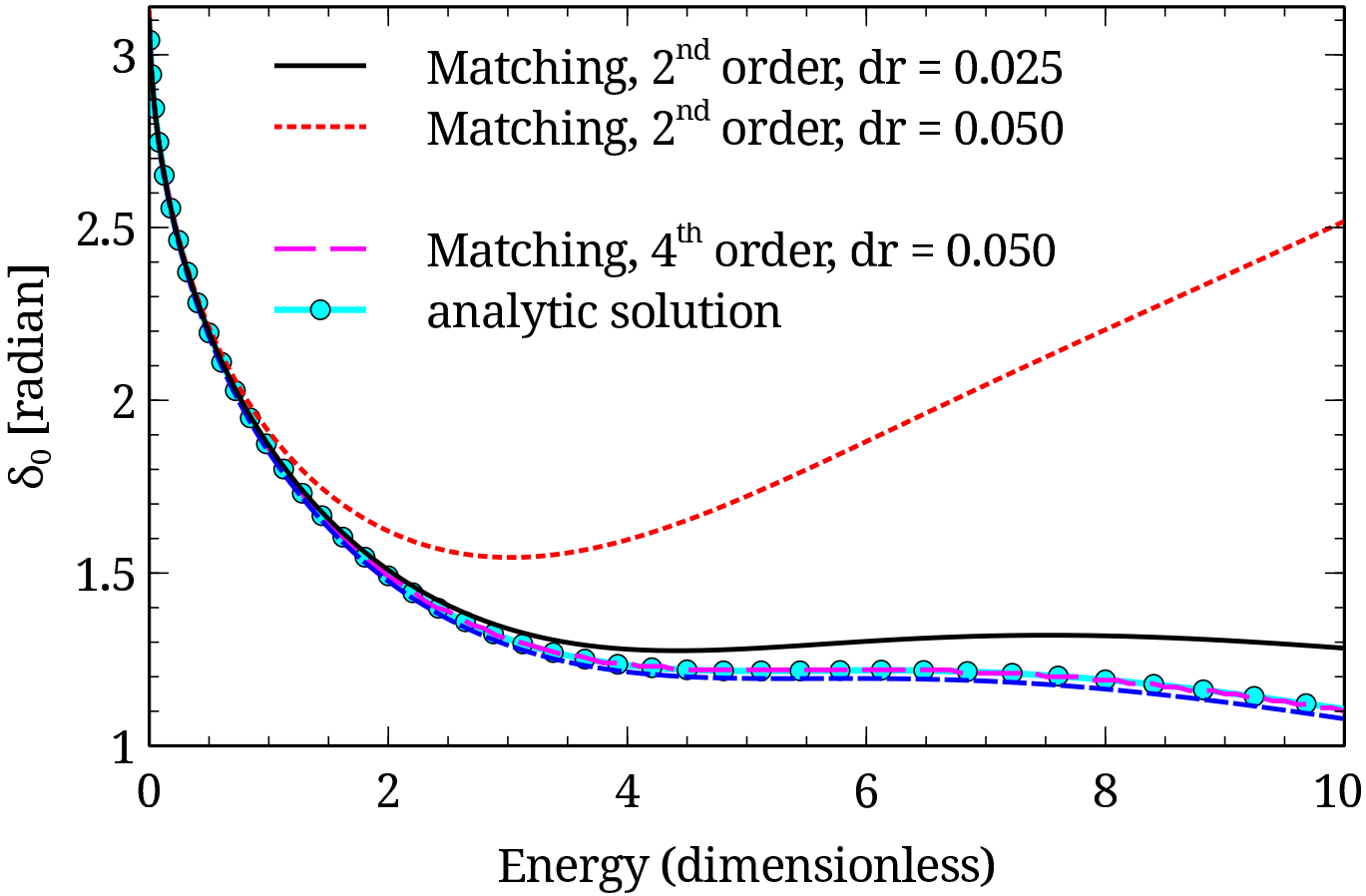

square well phase shift calculation

well radius = 1 unit

Scattering in a shell-model basis

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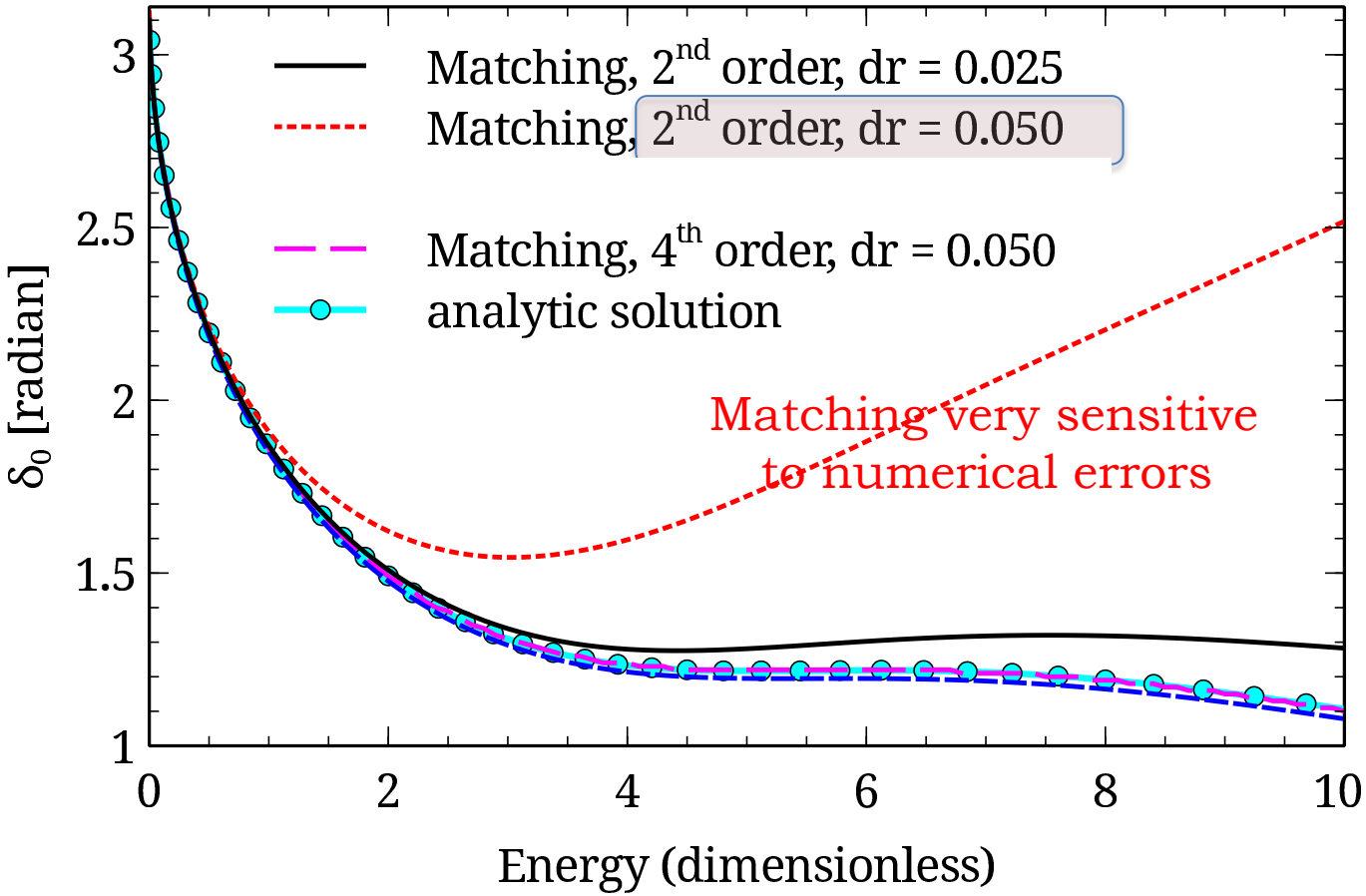

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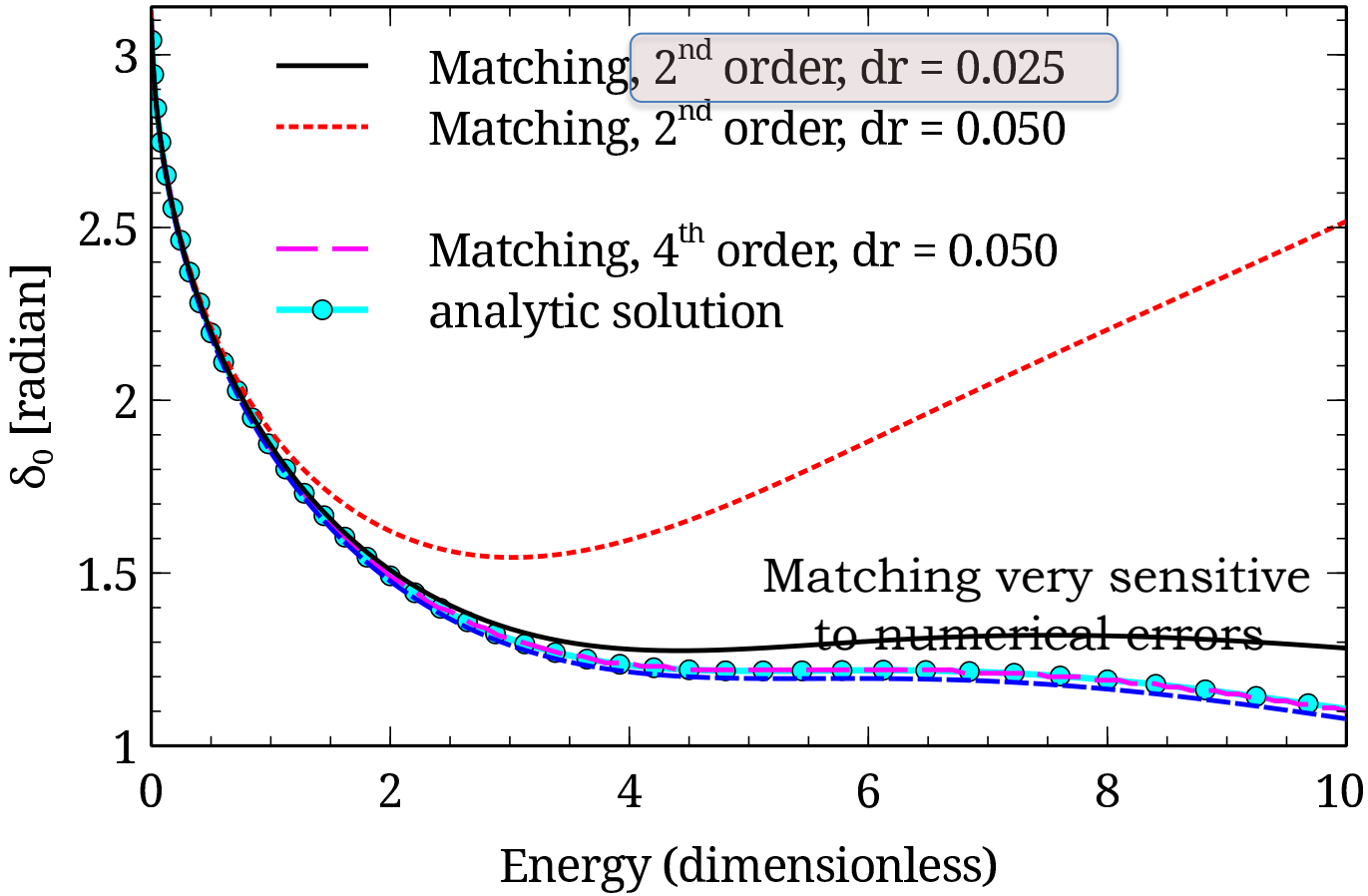

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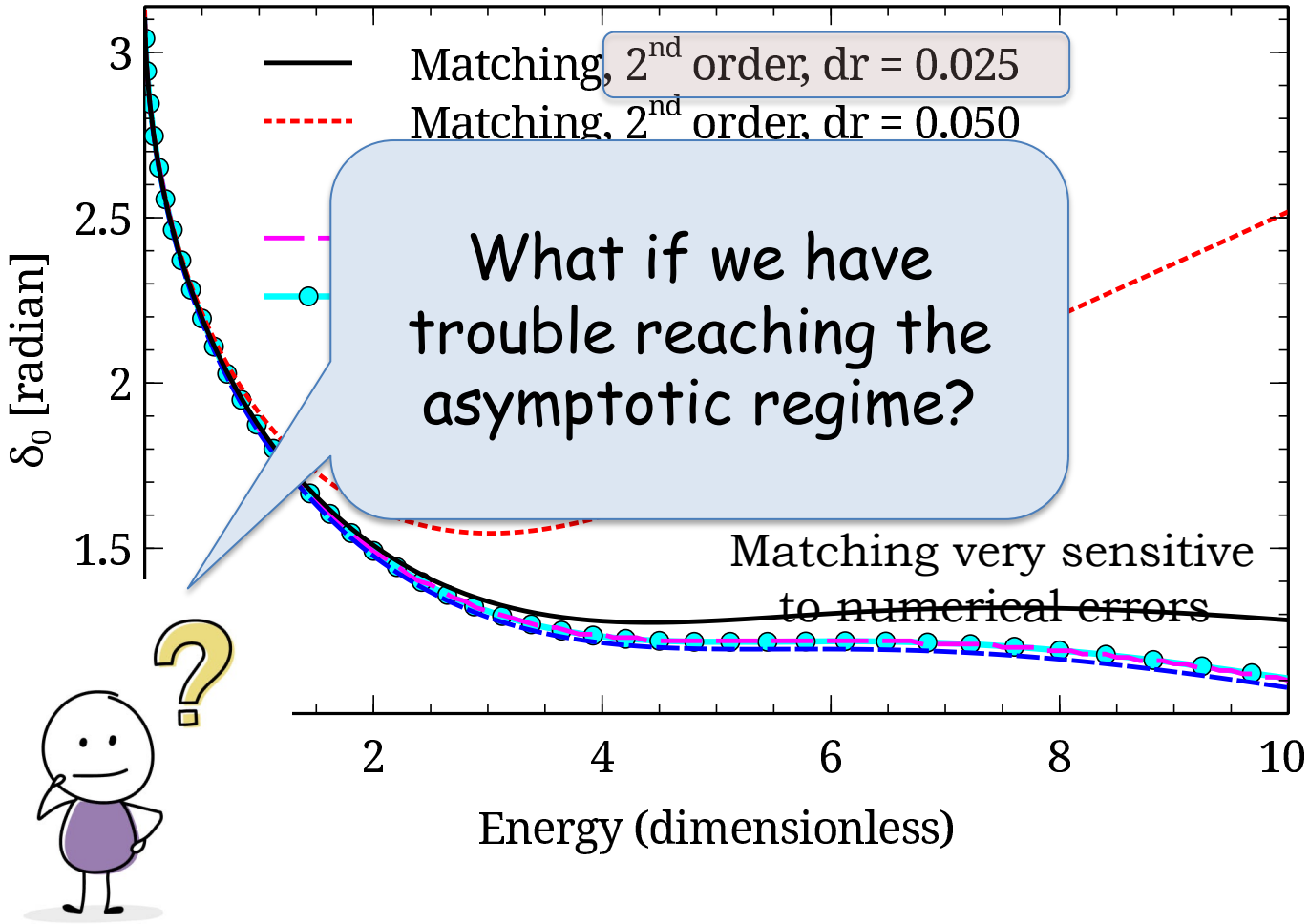

square well phase shift calculation

well radius = 1 unit

Math to the rescue!

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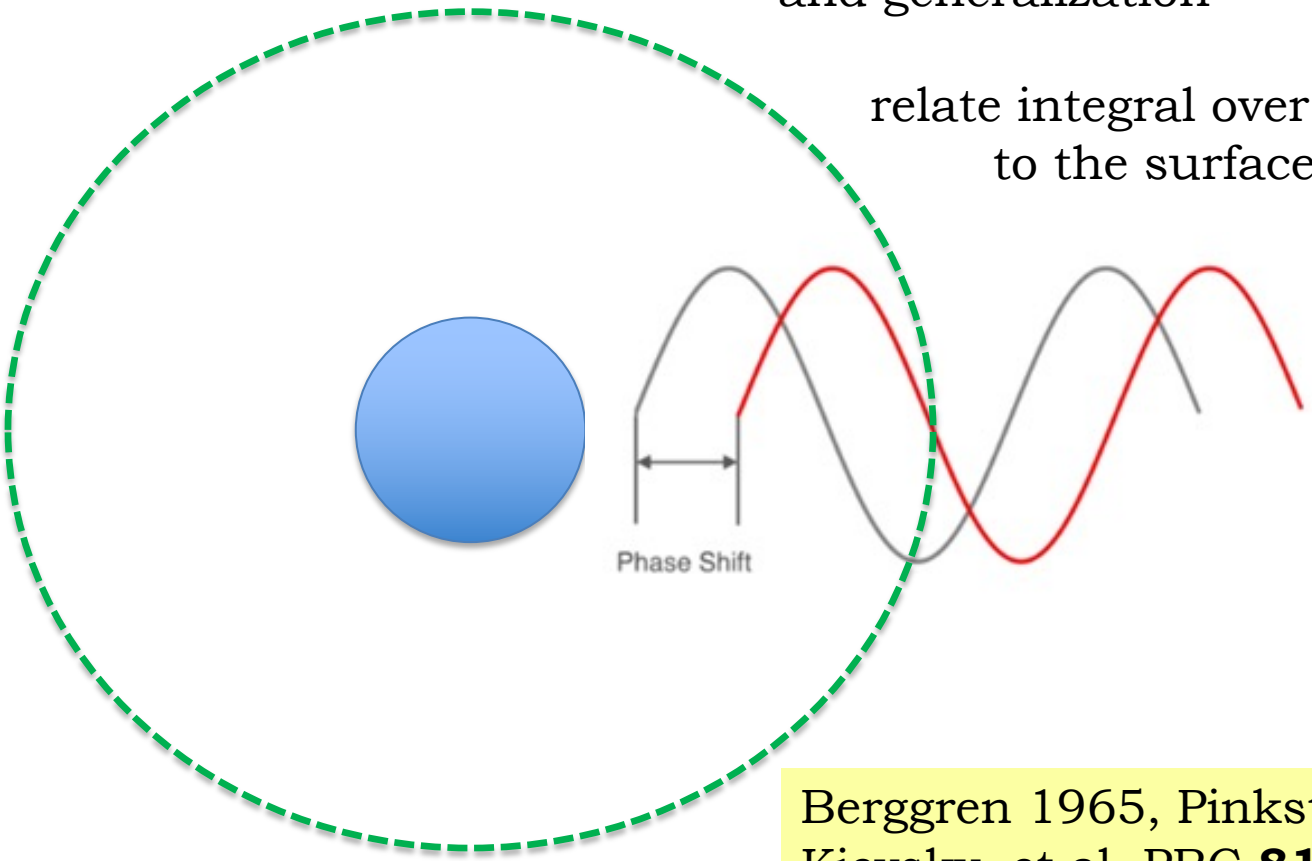
Green's theorem/Stokes' theorem
and generalization

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

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Extract phase shift/ S-matrix		Overlap/integral



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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

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

correction term (arises from inhomogeneous diff eqn)

irregular free scattering function

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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

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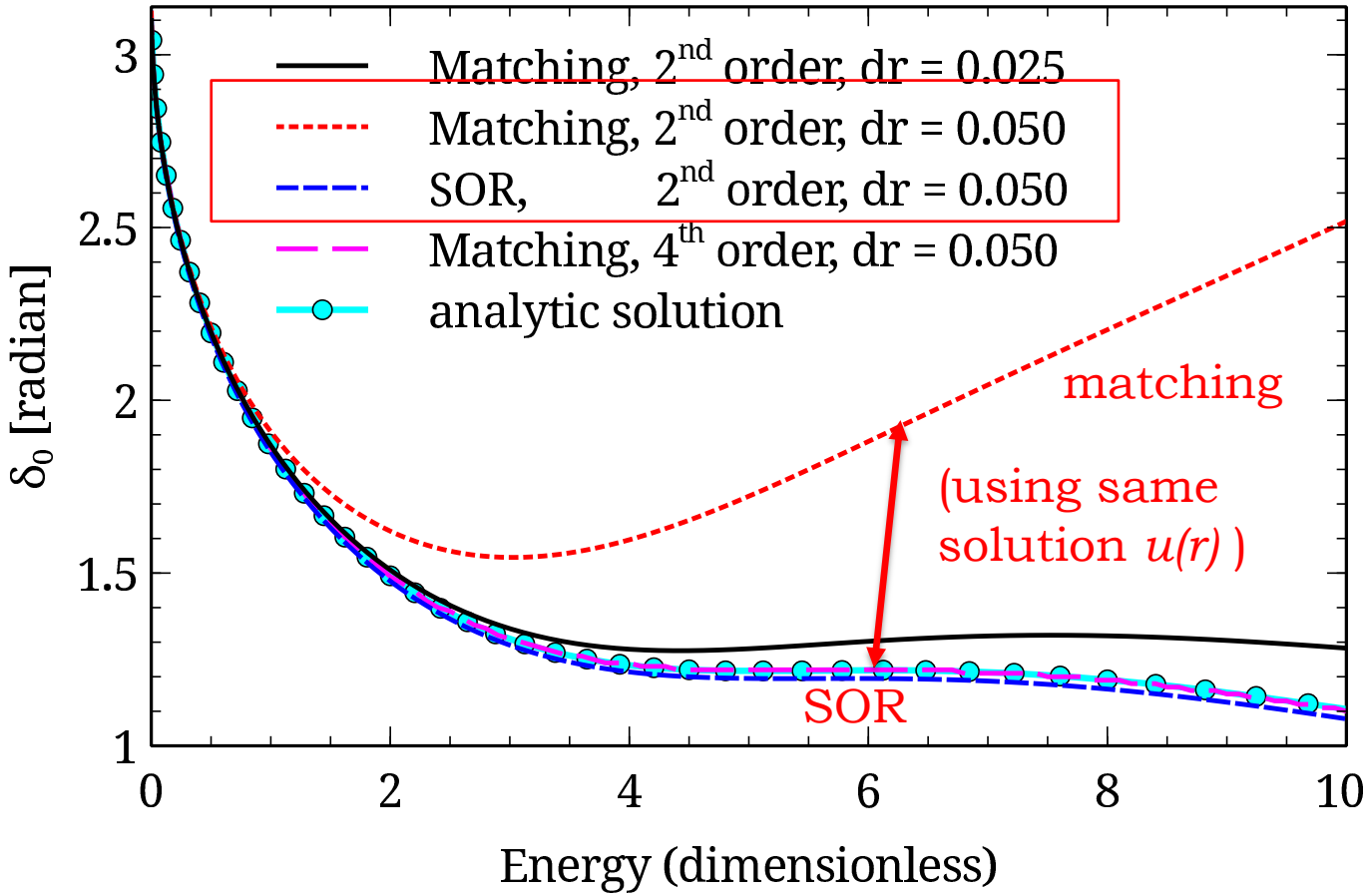

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Scattering in a shell-model basis

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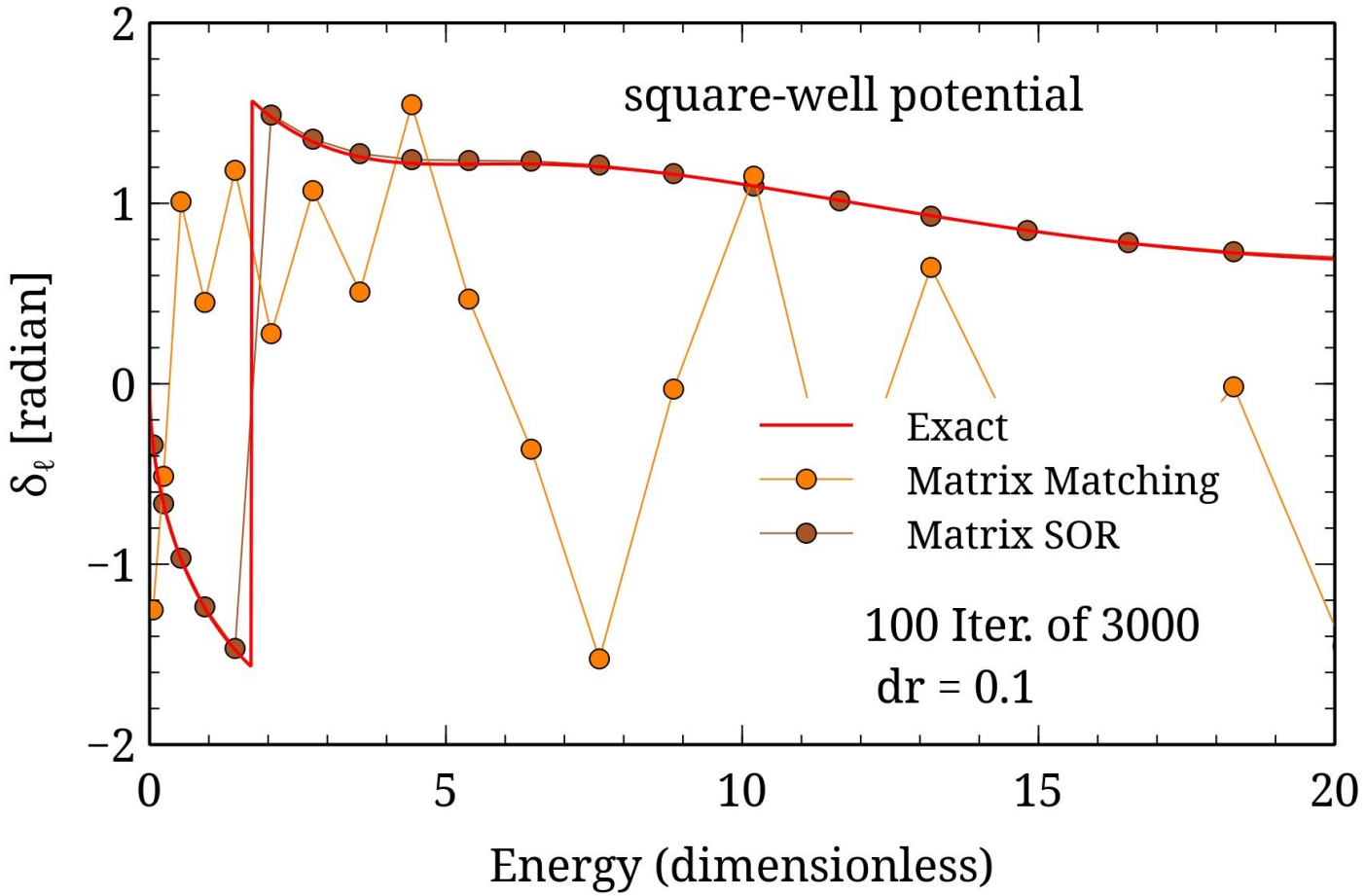

Approx calculation from Lanczos → Slow to converge at large *r*

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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.



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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)



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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" Heller & Yamani, PRA **9**, 1201 (1974))
which is congruent with no-core shell model
Cf. Shirokov *et al*, PRC **94**, 064320 (2016)

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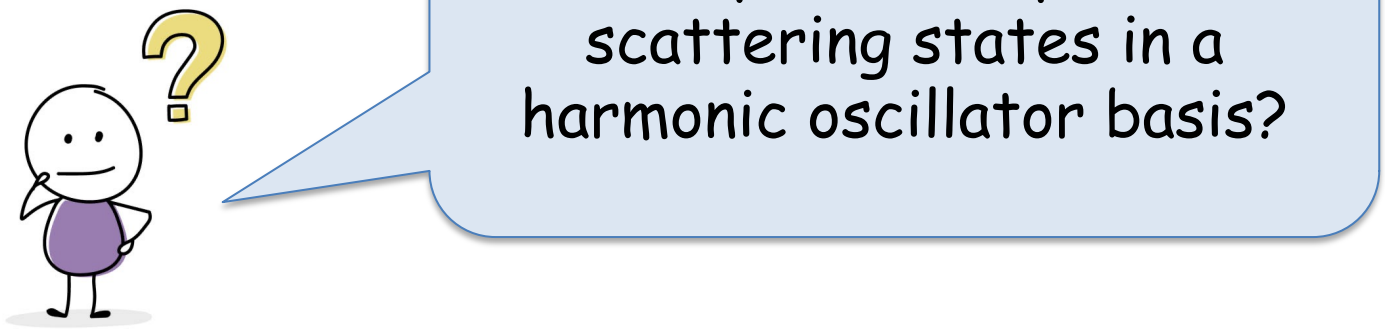
Cf. Shirokov *et a*



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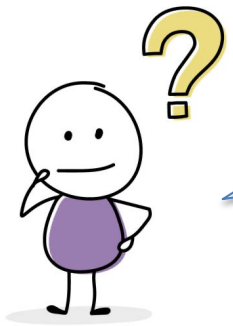

Wait, you can represent scattering states in a harmonic oscillator basis?

Yes!



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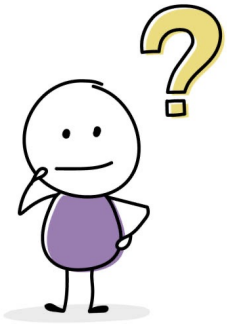
Consider the free (s-wave) regular function.
We can expand in a basis…

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





Scattering in a shell-model basis



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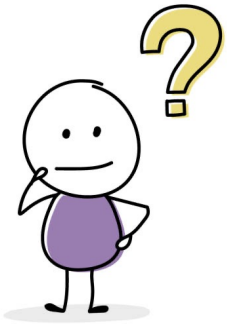
We can expand in a basis…

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

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))





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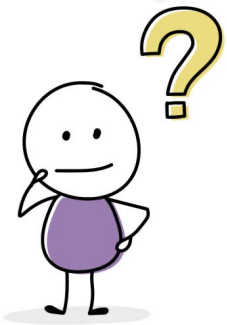
Consider the free (s-wave) regular function.
We can expand in a basis…

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

For oscillato… …nalytically.

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

But don't you need an infinite number of basis states?



Actually, no…



Scattering in a shell-model basis

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

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

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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**

- Convergence is slow, however, with model space

Scattering in a shell-model basis

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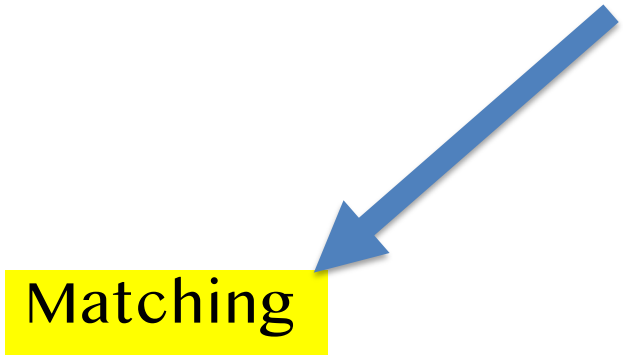
Standard Novel

Scattering State basis

Oscillator or other L^2-integrable



Extract phase shift/ S-matrix

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

however:
to get many energies requires many basis states

Computing

- One can … oscillator basis

("J-matrix … e shell model

Cf. Shirok… valent to **matching**

- Converg…





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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

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	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)

San Diego State University

Flow chart of project

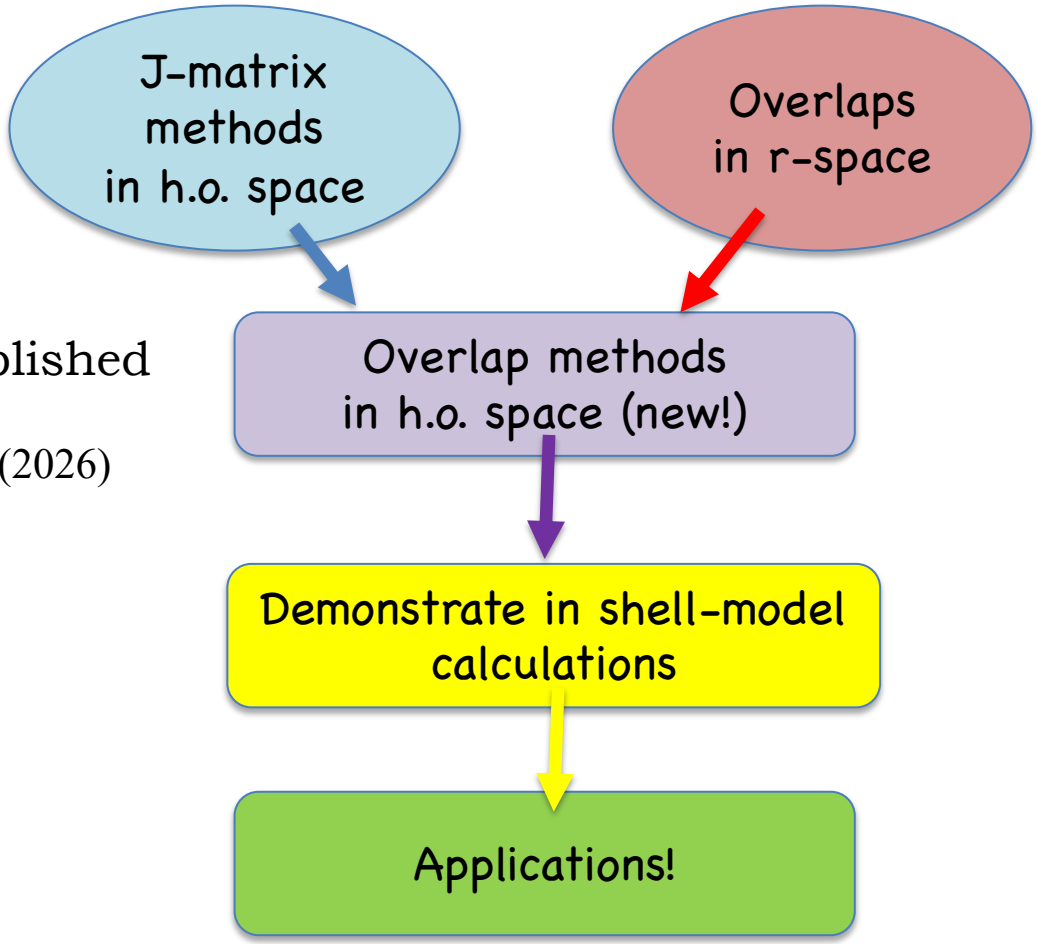
Input concepts:

Foundational paper published

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

In progress….

Near future



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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)

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We have generalized to finite bases

e.g., harmonic oscillator basis

"scattering overlap relation" = SOR

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

coefficient

basis function

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

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

basis function

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

correction term (arises from inhomogeneous diff eqn)

Scattering in a shell-model basis

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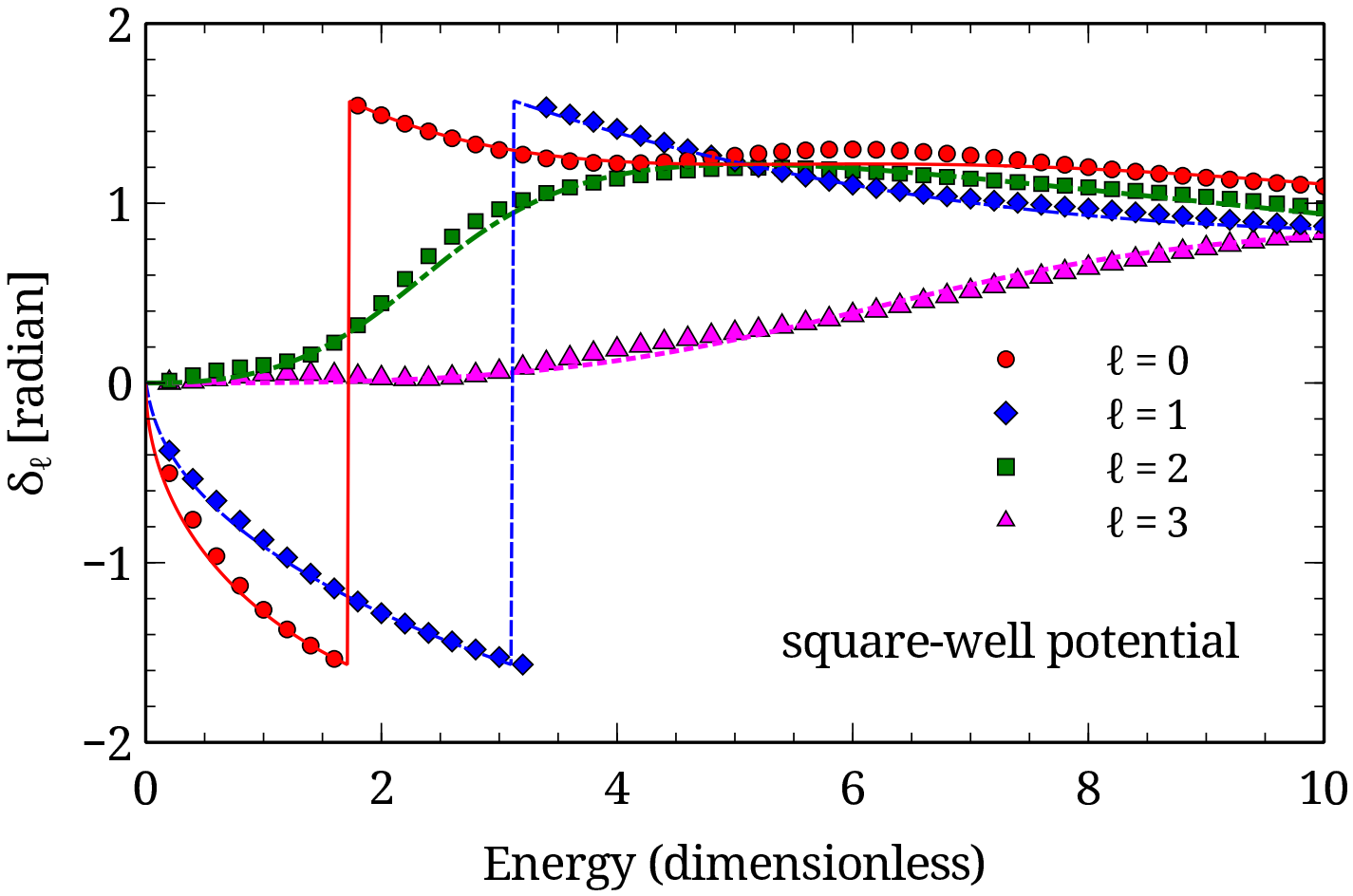
Full scattering solutions generated
via Lippmann-Schwinger at any energy



Scattering in a shell-model basis



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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.

The resolvent can be computed in shell model via Lanczos

(implemented and soon to be tested)

Scattering in a shell-model basis

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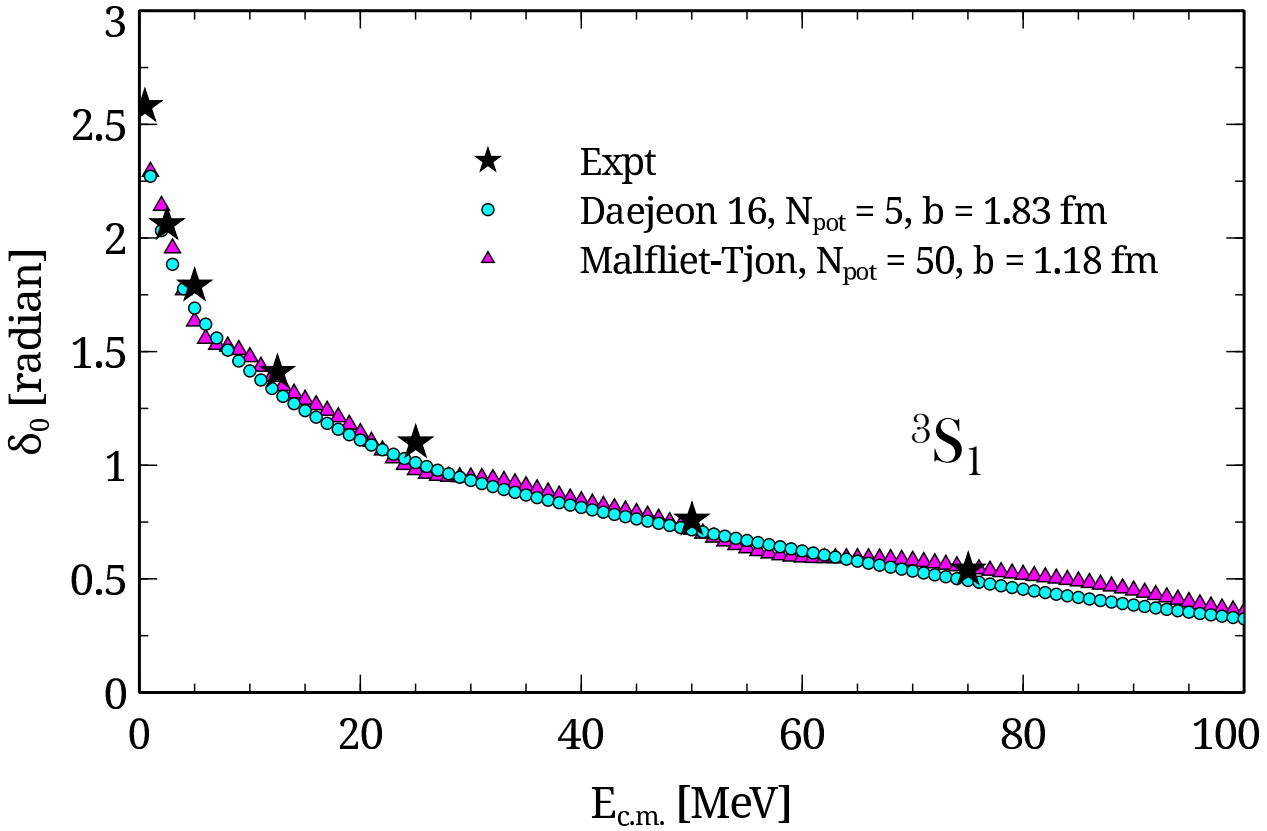

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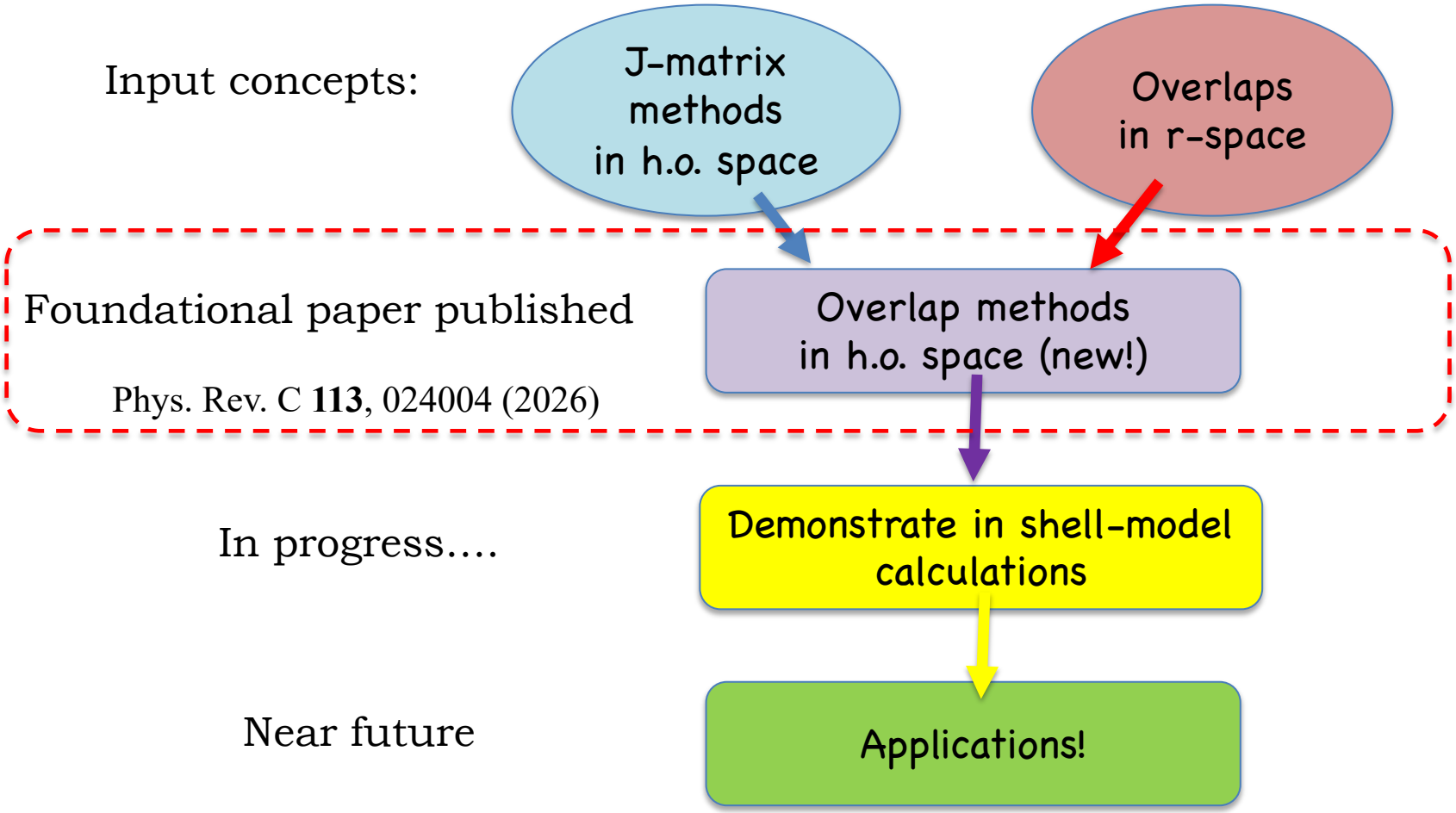
Flow chart of project





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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…)



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Recent Work

- Extension to coupled-channels S-matrices
- Moving towards implementation in shell-model
- (Developed formalism for generalized bases, incl. Coulomb)

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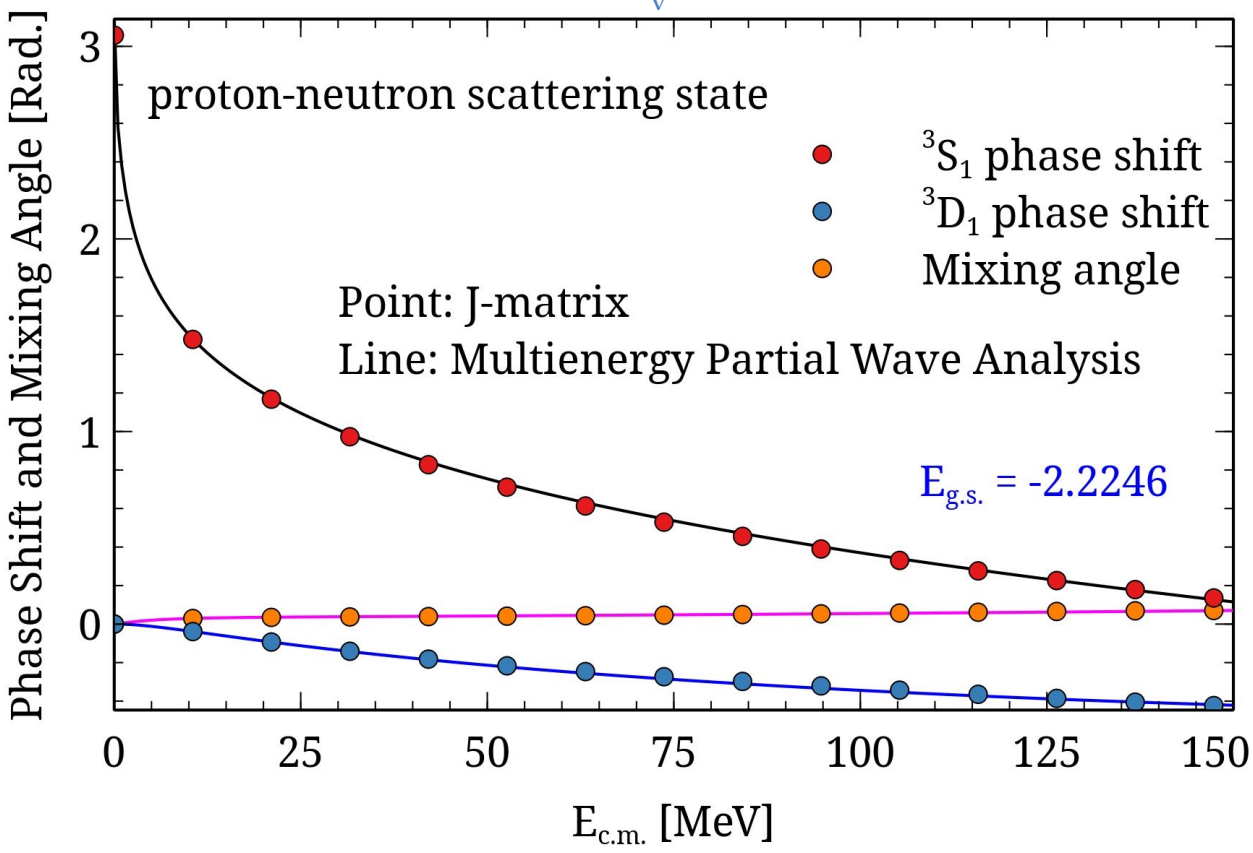
In progress

- Generalization to coupled-channel S-matrices



Preliminary



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Towards shell-model implementation

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



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Towards shell-model implementation

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

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

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Towards shell-model implementation

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

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

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Towards shell-model implementation

This is an effective potential due to the frozen target (^{4}He, ^{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

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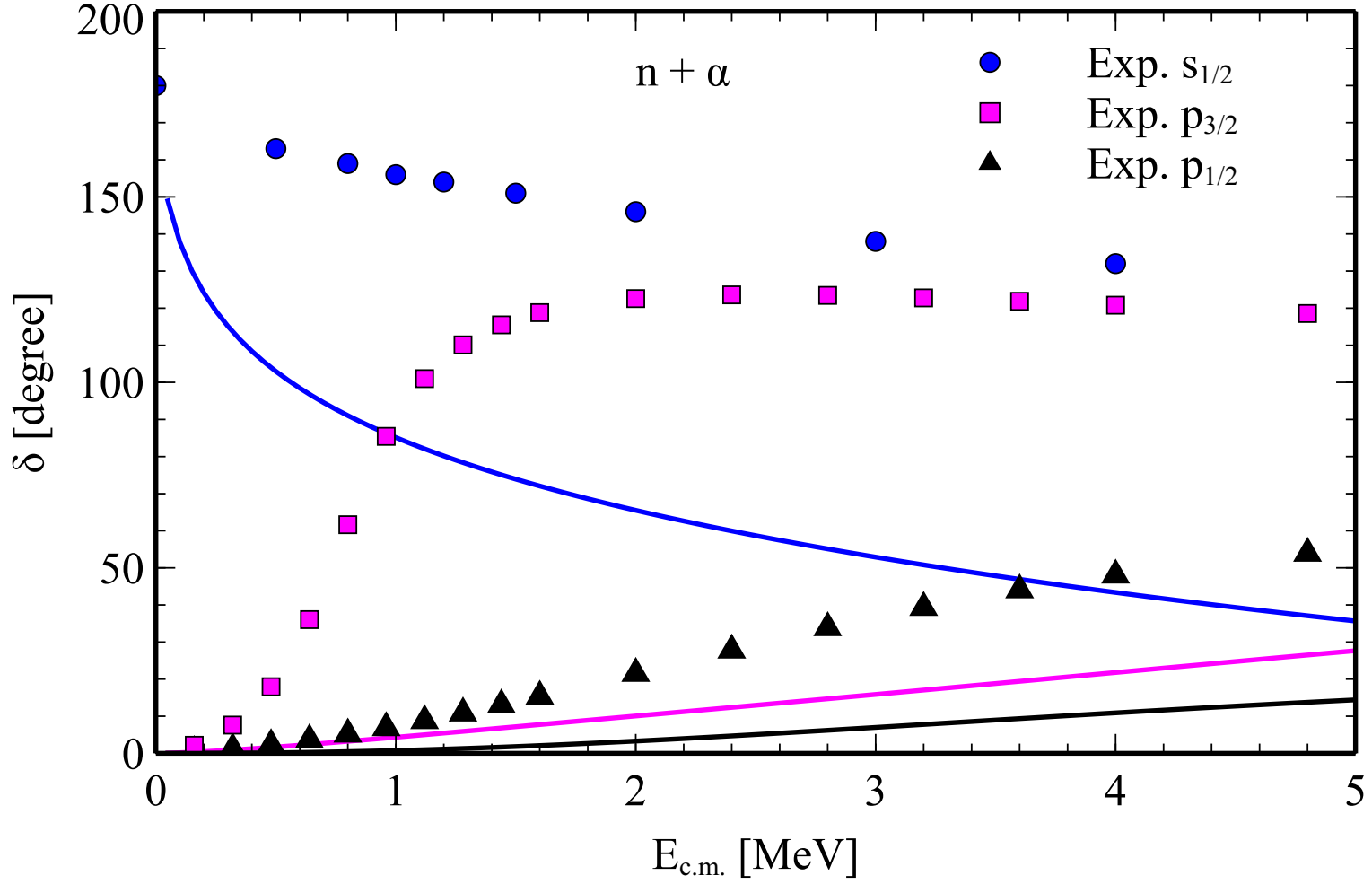
Preliminary



Scattering in a shell-model basis

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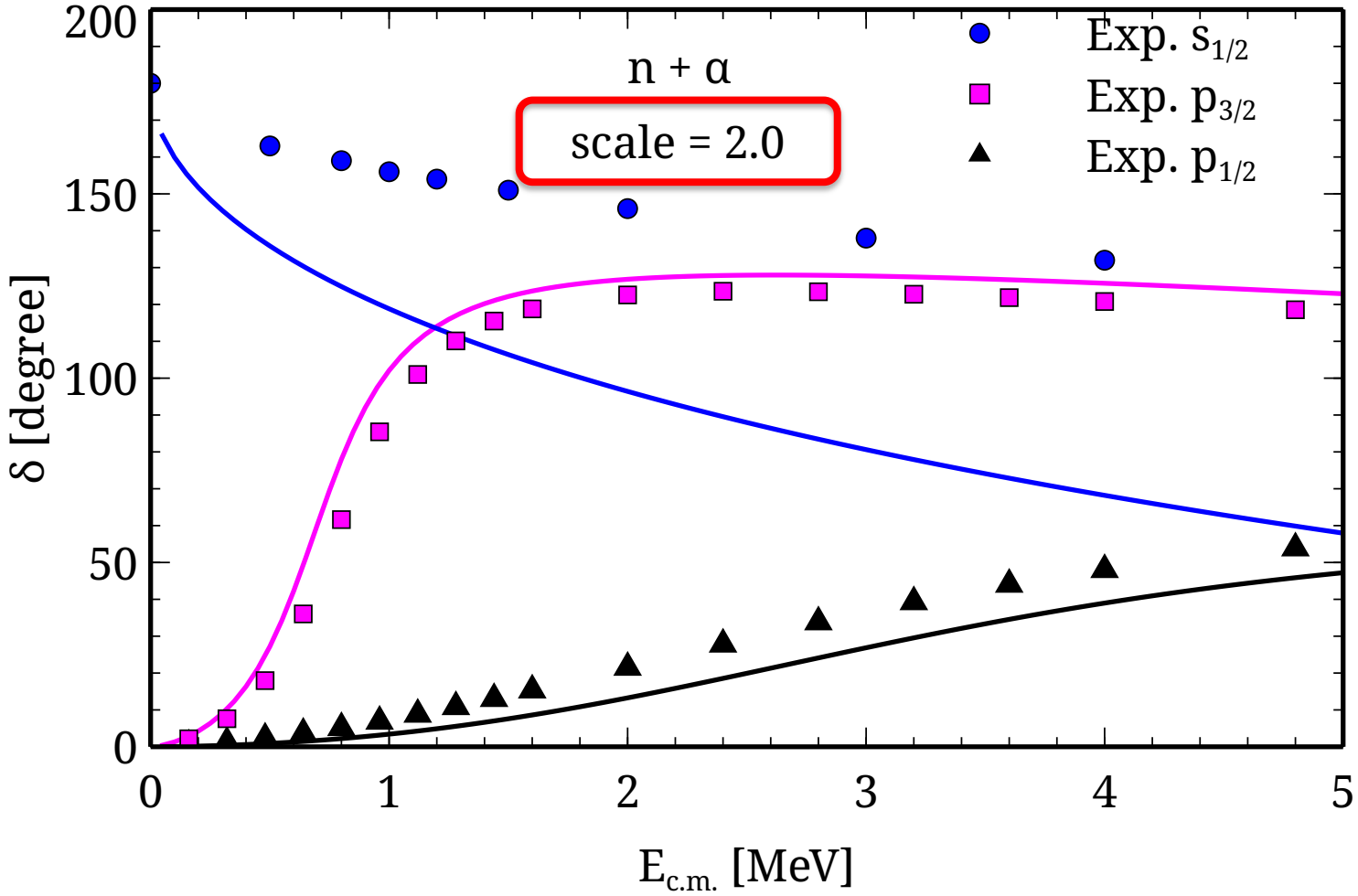
Preliminary



Scattering in a shell-model basis

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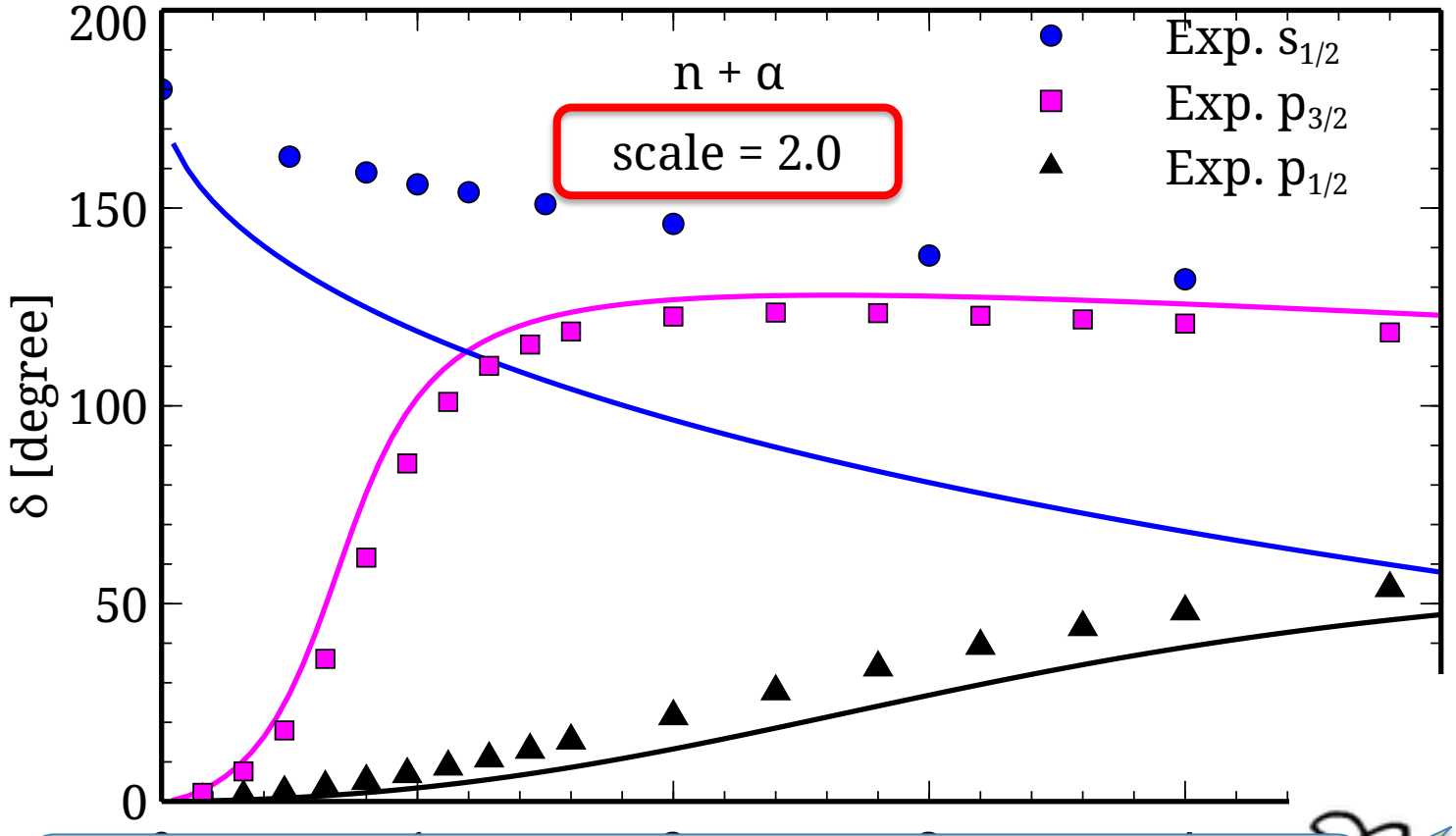
Preliminary





Not realistic, but interesting!

Scattering in a shell-model basis

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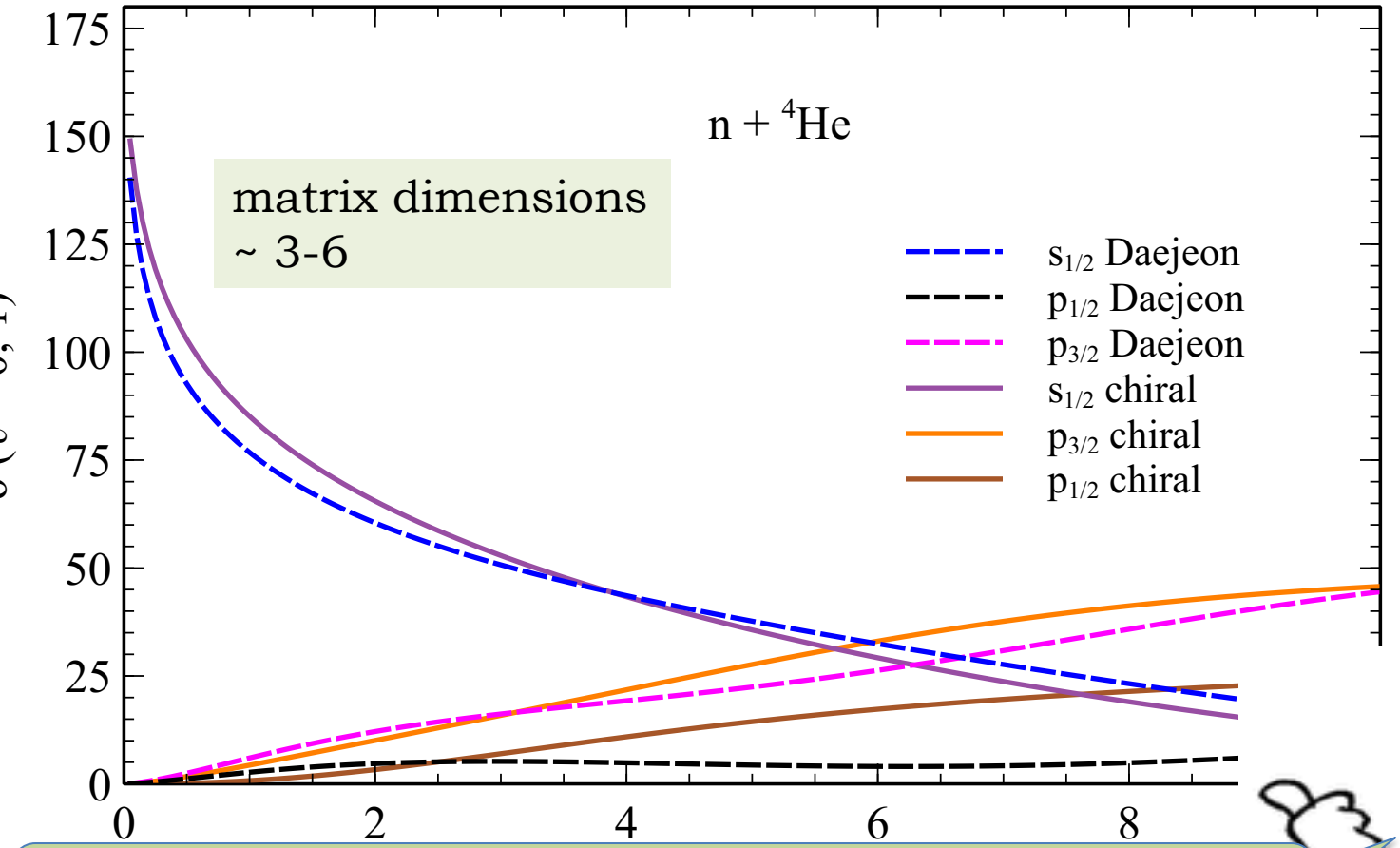
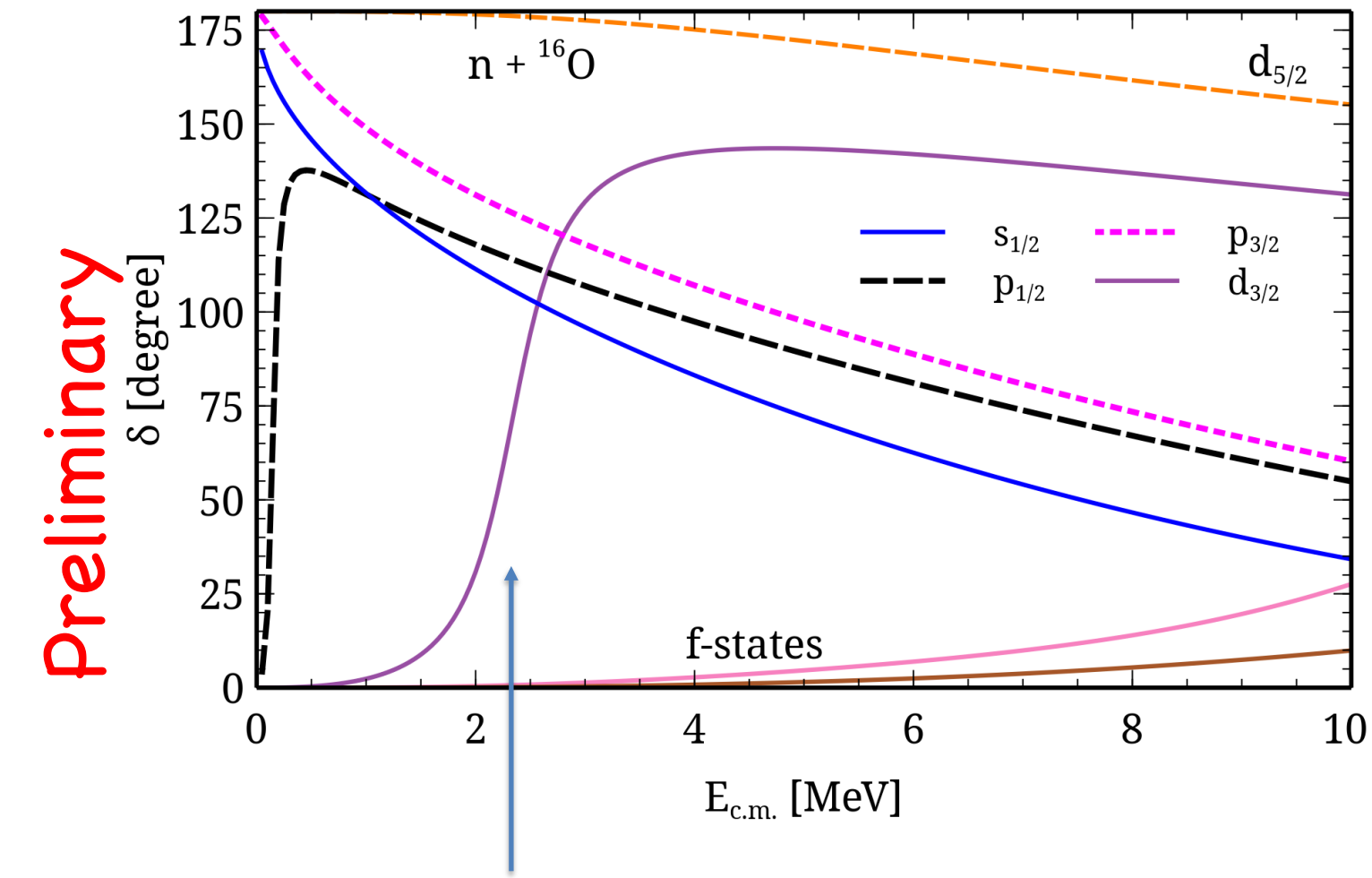
Preliminary





Not very sensitive to force!

Scattering in a shell-model basis



Note $d_{3/2}$ resonance, also seen in other calculations



Scattering in a shell-model basis

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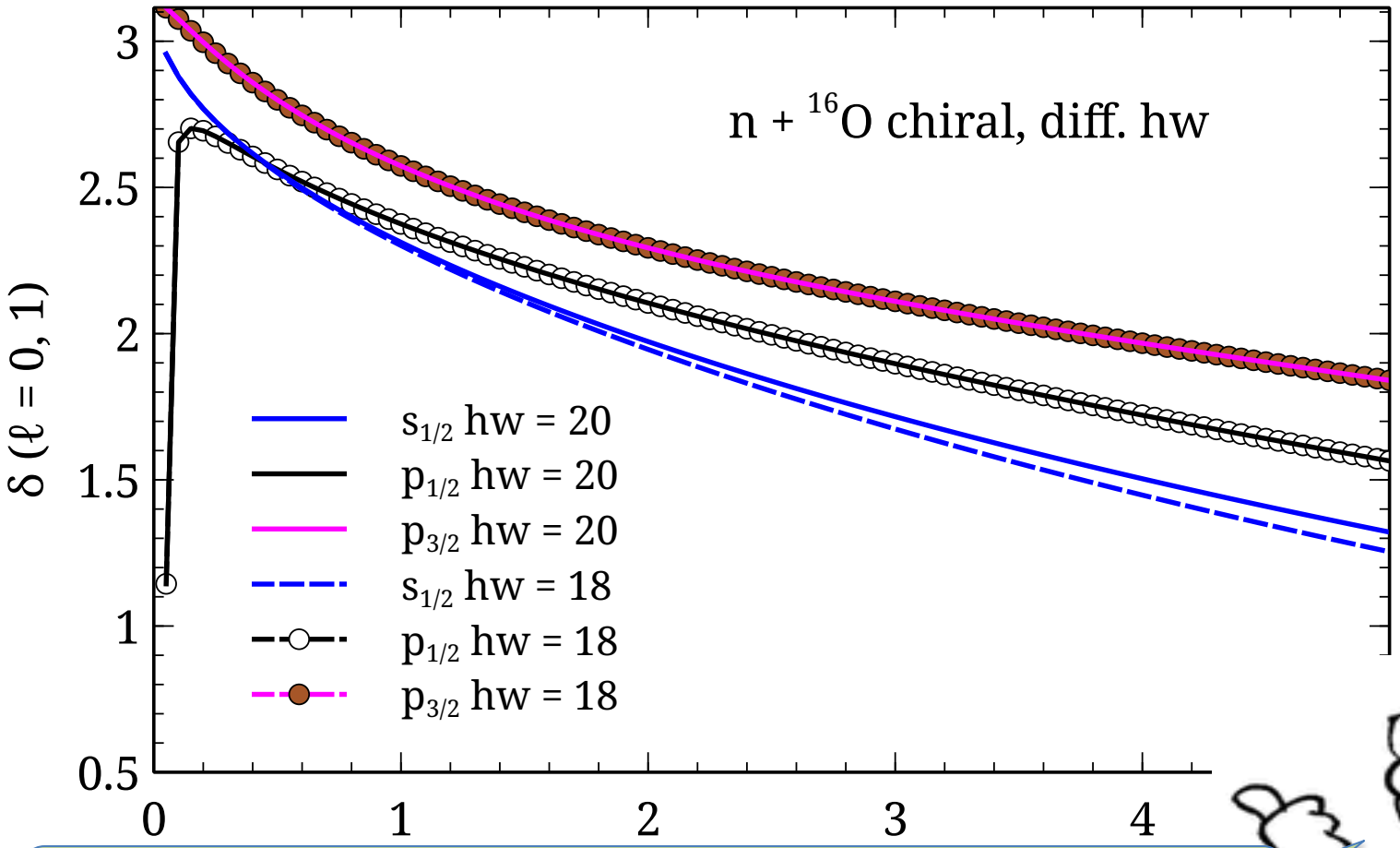
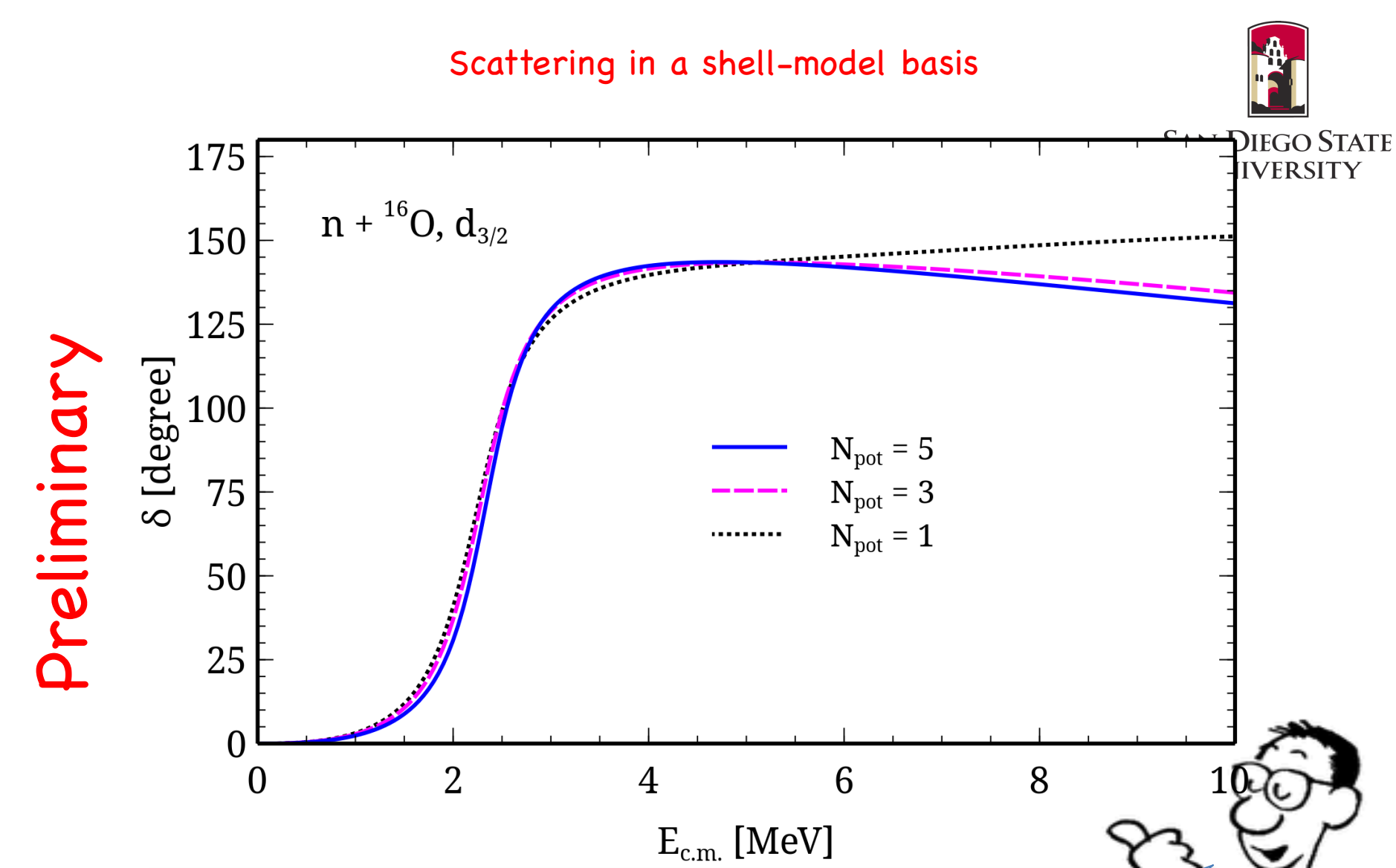
Preliminary





Not very sensitive to basis frequency!

Scattering in a shell-model basis



Not very sensitive to basis dimension!

Scattering in a shell-model basis

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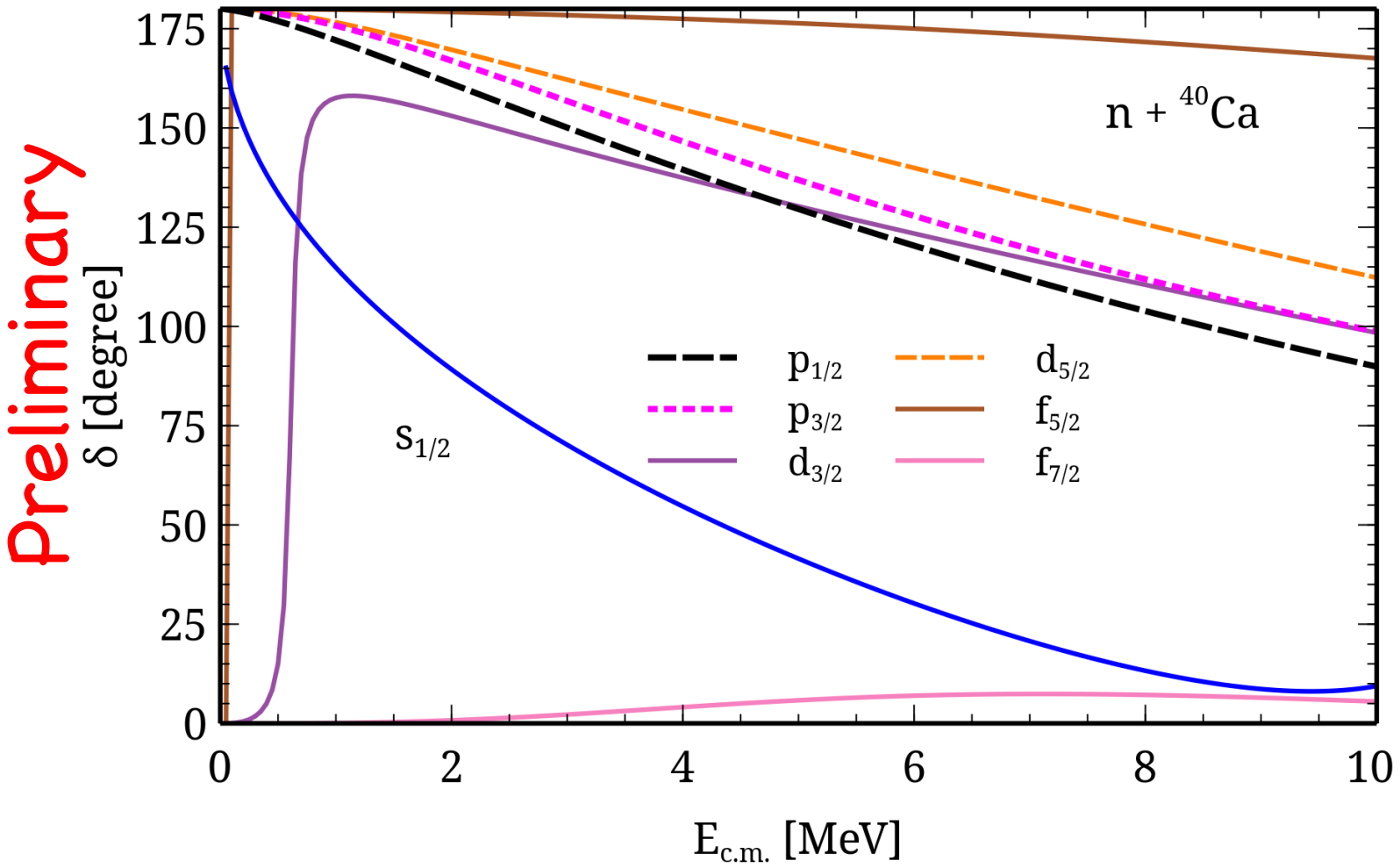



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Now that we have this as potential scattering,
we can redo in a shell-model code,
keeping the core frozen.

Then we can unfreeze the core for a fully dynamic calculation

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What would a full NCSM calculation look like?

1. Generate target g.s. | $A_{g.s.}$ >, using shell model code
(can use excited states for open channels)

2. Attach a 'free' scattering nucleon,

$$|u_{free}(k)\rangle = \left(\sum_n f_n(k)\hat{a}_n^+\right)|A_{g.s.}\rangle$$

(code for this exists)
(can do for both regular and 'irregular')

3. Apply Lippmann-Schwinger to get full scattering solution

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

(code for this exists)



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What would a full NCSM calculation look like?

4. Project out scattering states with good center-of-mass (we already do this routinely with Lanczos projection)

(4a) If more channels are needed—e.g., excited target states—this is straightforward to do.

5. Then compute $\langle u_{free}|V|u_{scatt}\rangle$ (code also exists)

We hope to *finally* do this during the summer!

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Next steps

- More general bases, and Coulomb scattering (formalism done)
- Asymptotic normalization coefficients (formalism in progress)

+ extension to reactions

- Applications: no-core shell model (start with n + ^{4}He)… valence shell model?
- Can we find poles/resonances/compute widths?



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What about statistical reactions?

(very briefly)

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What about statistical reactions?

One can provide a statistical representation of shell model Hamiltonians and operators as *partitioned random matrices*

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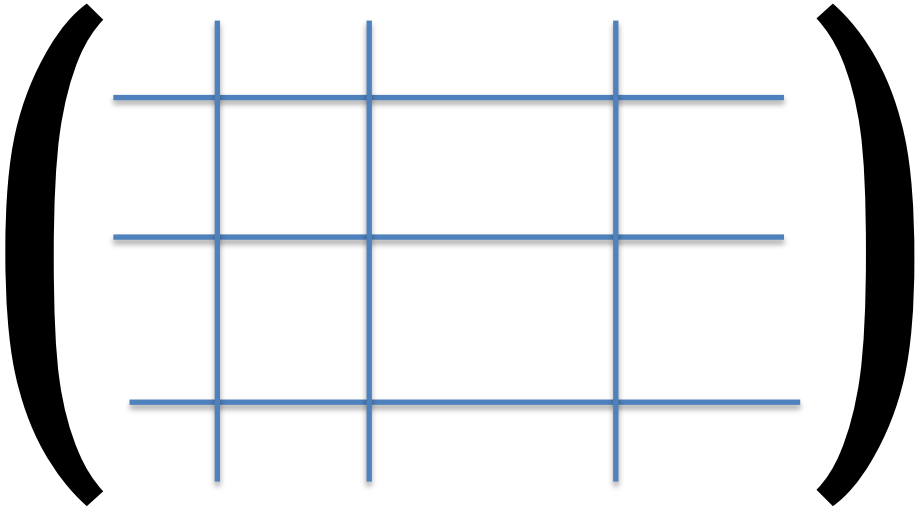
What about statistical reactions?

One can provide a statistical representation of shell model Hamiltonians and operators as *partitioned random matrices*



replace detailed matrix elements

by random elements constrained 1st and 2nd moments

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What about statistical reactions?

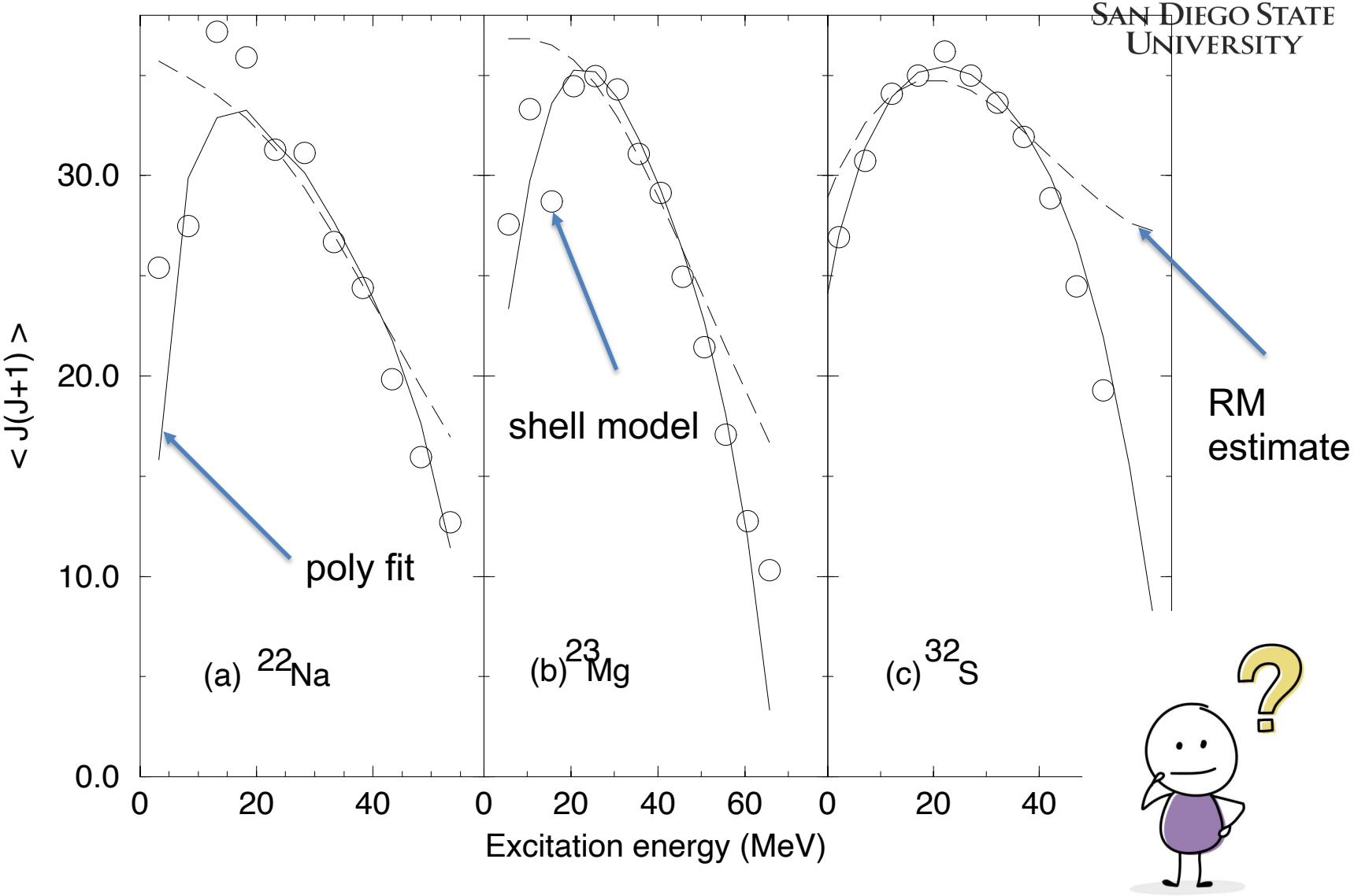
One can provide a statistical representation of shell model Hamiltonians and operators as *partitioned random matrices*

Advantage: can quickly carry out approximate calculations in much larger spaces than otherwise possible (of, e.g., level desnity)

Disadvantage: density of states of a GOE random matrix is semi-circle, not Gaussian → description of tails (low energies) is terrible

But at higher excitation energies, works reasonably well

Scattering in a shell-model basis





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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 shell-model (or other many-body) calculations

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What I'm hoping for:

Collaborators/partners interested in further development/applications:

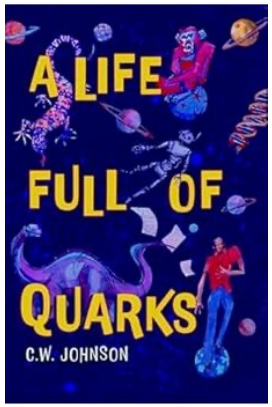
- Apply to shell-model / other many-body methods
- Apply ANCs to reactions

Alternate way to solve coupled channels

Also:

- Extend to RGM? To Faddeev?







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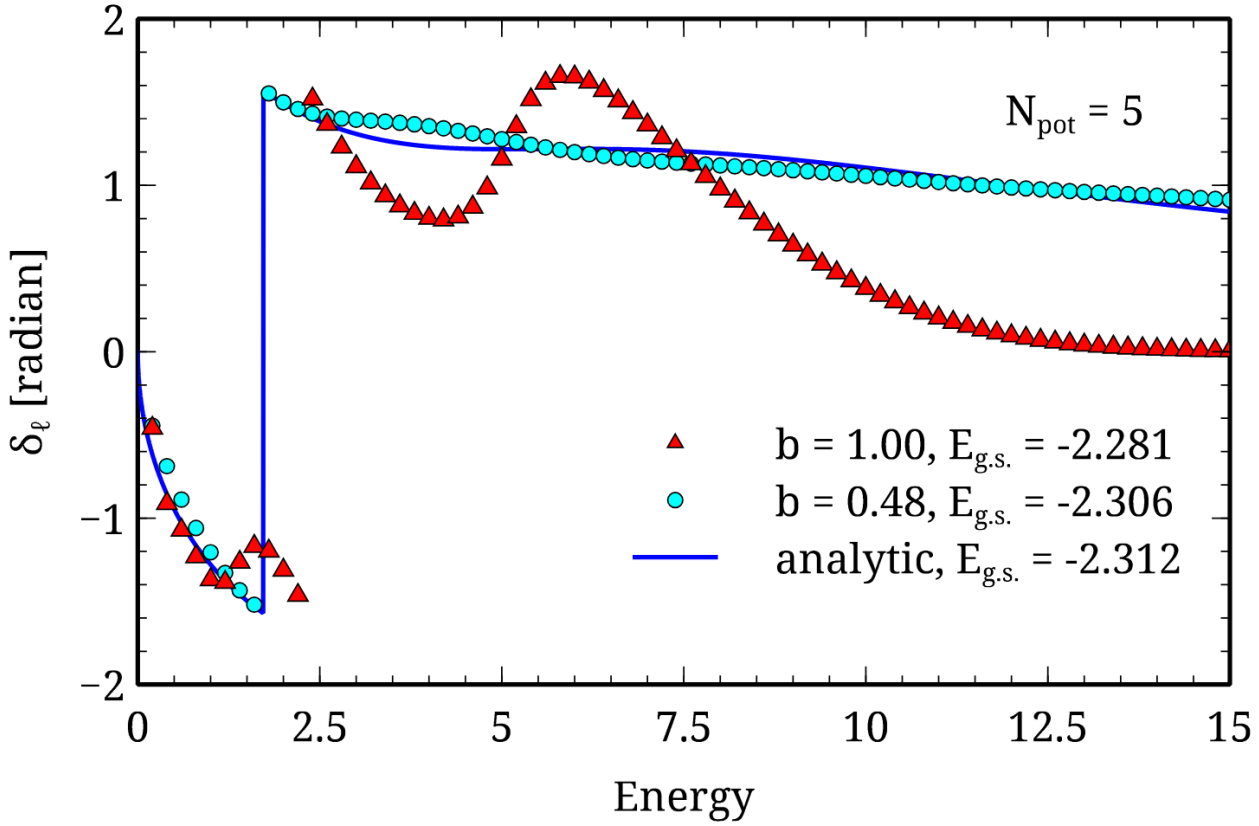
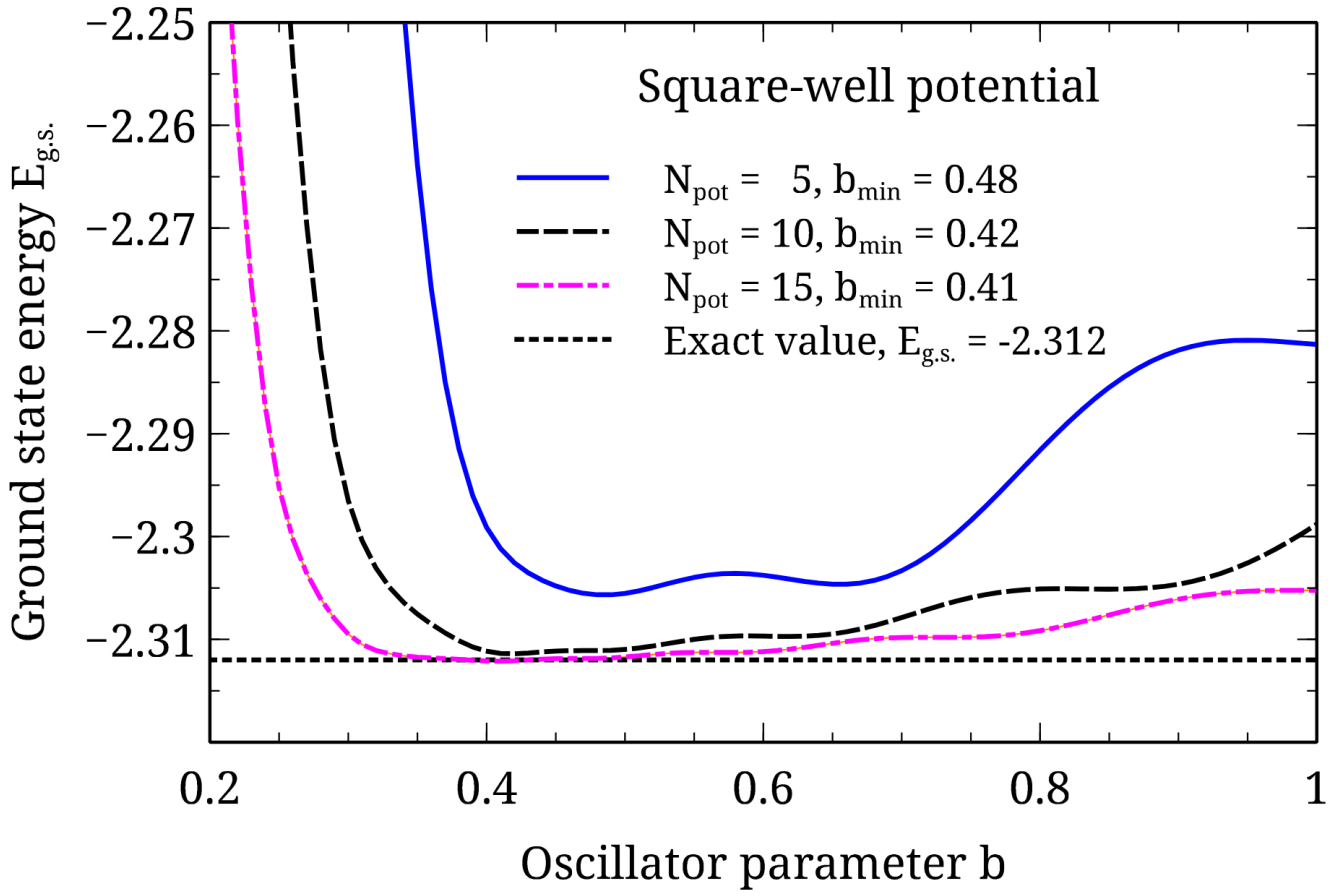
Extra slides

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

Some notes on derivation of SOR in coordinate space

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

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

Here, u_{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



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

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

Representation of free functions in finite basis



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

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

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

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