An overview of *ab initio* scattering, reactions, and operators (circa 2014)

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My agenda today

I know nothing about T violation, except that no one ever seems to go back in time

I told Vladimir I'd review *ab initio* methods as they apply to scattering & reaction observables

I'll also talk a little about the kinds of operators (strong & electroweak) in use, because it seems relevant here

There's a lot more going on than what I keep up with

What follows will be a review of some things that I think are either important or likely to be of interest to this audience

Things that I sort of understand will be overrepresented
(and I assume you can find papers without explicit reference)

The *ab initio* program: One man's view

Ab initio: Latin "from the beginning"

The idea is to compute nuclei as collections of interacting nucleons

The interaction should be the same one measured in NN scattering

A successful *ab initio* theory of nuclei requires accurate interaction & accurate computational methods

The payoffs (not linearly independent):

Quantitative comparison with a broad range of experiments

Reliable application to astrophysics & technology where there's little data

Probing small interaction terms (3-body; P, T, or T violating)

Another turtle below this one?

"The beginning" ought in principle to be quarks & gluons, but that's difficult

There is work being done to compute a nucleon-nucleon interaction on the lattice

It's still far from the physical pion mass, which is a show-stopper for most nuclear physics – π exchange is important

Proponents of computing nuclei from lattice QCD occasionally admit that the m_π difficulty will limit what they can usefully do

Demonstrated failure of the nucleon-level model would be interesting, but you really have to nail the computational aspects before calling it a failure

The basic NN interaction

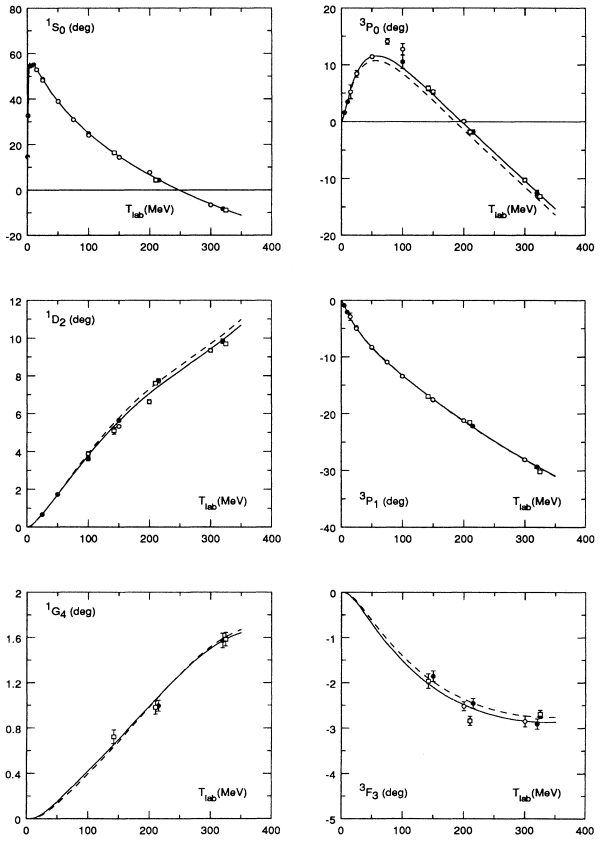
"Realistic" *ab initio* models are based on an NN interaction that reproduces NN scattering observables up to $E \approx m_\pi$ (& ^{2}H properties)

So far this has meant reproducing the Nijmegen phase shift analysis

(Lots of weeding & cleaning up of data)

Smooth phase shifts required:

- consistent data
- explicit one-pion exchange
- small corrections to the EM potential: vacuum polarization, magnetic moments...



Stoks et al. (1993)

Several representations of the potential have been fitted with $\chi^2_\nu \approx 1$:
Nijmegen I & II, Reid 93, CD Bonn, Argonne v_{18}, N^{3}LO chiral

What an NN interaction looks like

A good NN interaction, like a good story, has a beginning, middle, and end

Long range ($\gtrsim 1.5$ fm) looks like one-π exchange (tensor term important)

Medium range ($\gtrsim 0.5$ fm) has a complicated operator structure in spin & isospin

Short range has strong repulsion

No matter what you do, you end up with ~ 40 parameters fitted to NN phase shifts (~ 18 operators, as in Argonne v_{18})

The operators have been organized in several ways to get different interactions ("empirical" operators, meson exchange, χEFT)

Multiple approaches get to $\chi^2_\nu \sim 1.0$

NN interactions: practical aspects

Traditionally, the largest sources of computational difficulty were strong short-range repulsion & rich operator structure (esp. tensor term)

These required enormous model spaces in basis methods (e.g. no-core shell model)

Quantum Monte Carlo allowed E calculations from good variational guesses built from the potential: no basis, so no convergence problem

But only Argonne-Illinois approach with "phenomenological local operators" had favorable forms for use with quantum Monte Carlo

Green's function Monte Carlo (but not variational Monte Carlo) has trouble with some types of momentum-dependent terms (often designed into χEFT)

There's finally progress on this front, both to work around "bad" potentials & to avoid unnecessary "badness"

Evolving operators

The solution to the hard-core problem in basis methods is to soften the hard core of the potential with a cutoff while retaining phase shifts

This had a false (but important) start with $V_{\text{low } k}$ & is now done with similarity renormalization group (SRG)

You also pay for smoothed 2-body NN potential with induced 3- & more-body terms

It's extra computation, but you need 3-body terms even before evolution, & higher-body don't seem to become larger overall

The evolution is just solution of 1st-order ODEs, so it can be done as exactly as the original interaction was known

Evolving more operators

Electromagnetic current operators of at least Argonne-type potentials are close to what you'd guess after your 1st E&M course

2-body currents are needed for current conservation, but they're small unless there's cancellation: $i[H, \rho] = \partial_t \rho = \nabla \cdot \mathbf{j}$

This lets you cover $(e, e'p)$ to $E > m_\pi$, actually to surprisingly high E

If you SRG-evolve the strong force, you also must evolve the EM currents (or others that interest you)

There somehow has to be a reasonable starting point for this – the unevolved currents must be consistent with the unevolved NN interaction

Few-ish-body calculations

The calculation of substantial nuclei from "bare" NN interaction has been one of the great triumphs of the last 20 years

This is a large body of work on mainly bound states, following several methods:

Variational Monte Carlo (VMC) & Green's function Monte Carlo (GFMC) – collectively QMC (also AFDMC) – Pandharipande, Carlson, Pieper, Wiringa...

Ab initio no-core shell model (NCSM) – Navratil, Quaglioni, Vary, Barrett, Ormand...

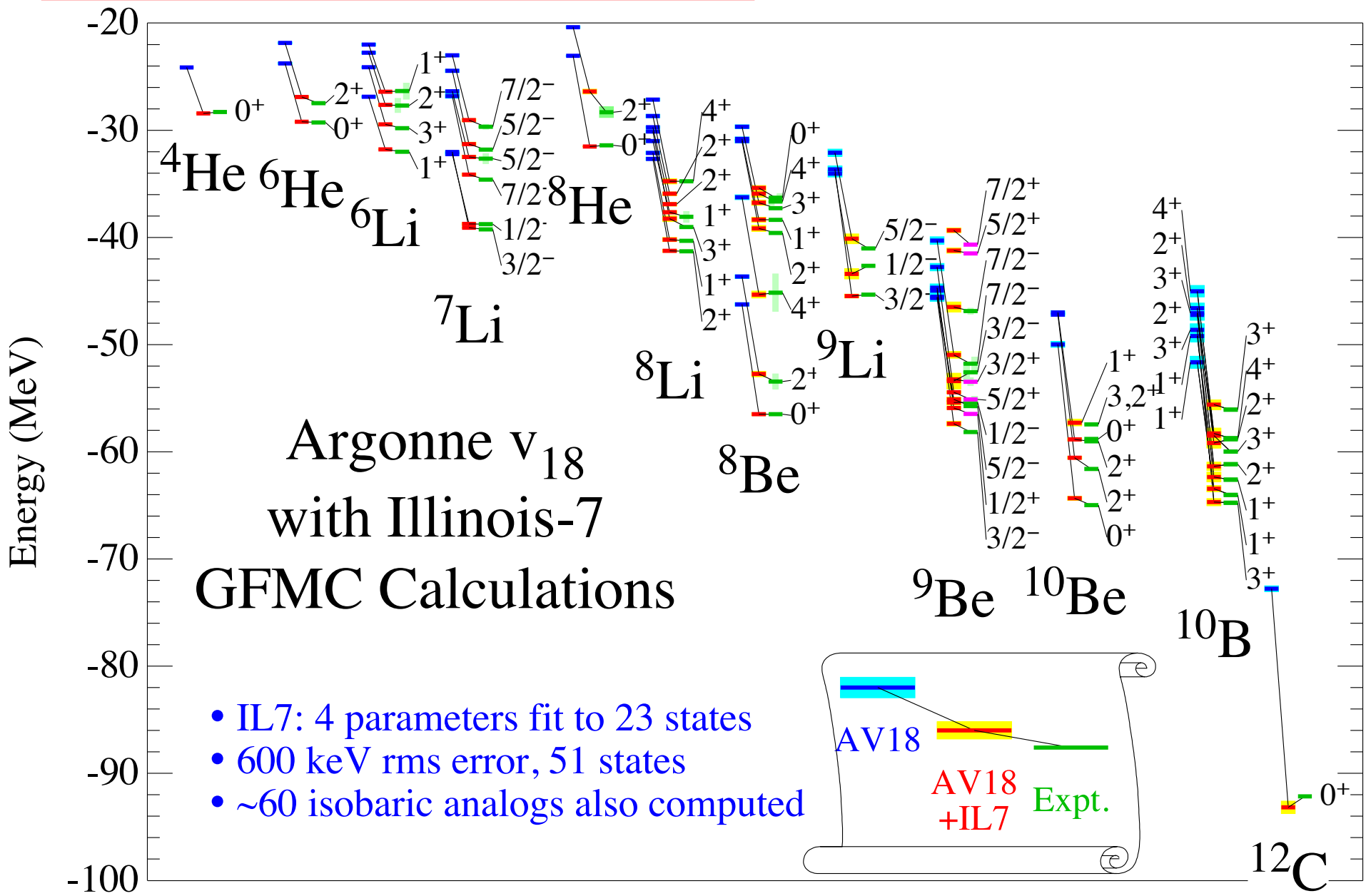
Coupled cluster (CC) – Hagen, Dean, Papenbrock...

Fermionic molecular dynamics (FMD) – Neff, Feldmeier

Lattice effective field theory (LEFT?) – Lee, Meißner...

In $A \leq 4$, there's also important work via Fadeev & related methods, and the correlated hyperspherical harmonic (CHH) basis

Energy spectra from quantum Monte Carlo



Well, actually...

The important points of that work:

Nuclear structure up to $A \gtrsim 20$ does indeed trace back to bare interactions

You can compute electroweak observables accurately with those wave functions

3-body terms (IL7 in the diagram) are important

At least in this collection of systems (& some higher masses with NCSM, CC, in-medium SRG), computational approximations are under control

(Some variation of computational precision with A, method, observable, inclusion of 3-body)

Strengths & weaknesses

As with anything in life, the best tool depends on the problem to be solved

QMC: Lack of basis is good for highly clusterized nuclei (e.g. ^{12}C) & weakly-bound states (if you can make good variational functions)

Each individual state requires human effort (not Lanczos diagonalization), lack of spatial basis can be unwieldy, problem grows fast with A

NCSM: Linear algebra in Slater determinants is powerful (Lanczos diagonalization of many states)

Clusterization & weakly-bound states difficult without further modification, 3-body forces take a lot of computation

CC: Scales very well with A but needs a closed-(sub)shell reference state

How do you extend that to reactions/scattering?

All of those methods naturally give you an eigenenergy & a square-integrable wave function

But reaction/scattering observables are S-matrix elements, not energies

Continuum wave functions are extended in r-space & highly clusterized

The natural extension is to compute wave functions in a finite volume & match across the boundary to get the S-matrix

You need a basis that can handle extended & clusterized wave functions

Even if the quantity that interests you can be handled by Fermi's golden rule, explicit continuum states are intermediate steps

Example: QMC in the continuum

Scattering calculations with QMC methods have been based on a particle-in-a-box formalism

The wave function is computed only within a (spherical) box defined by a cluster-cluster separation

Forcing $\Psi = 0$ or $\partial_r \Psi = \gamma \Psi$ at the surface, $H\Psi = E\Psi$ has a discrete spectrum

VMC or GFMC most easily gives the ground state energy at the chosen γ & box radius

You get phase shifts δ_{JL} by matching onto

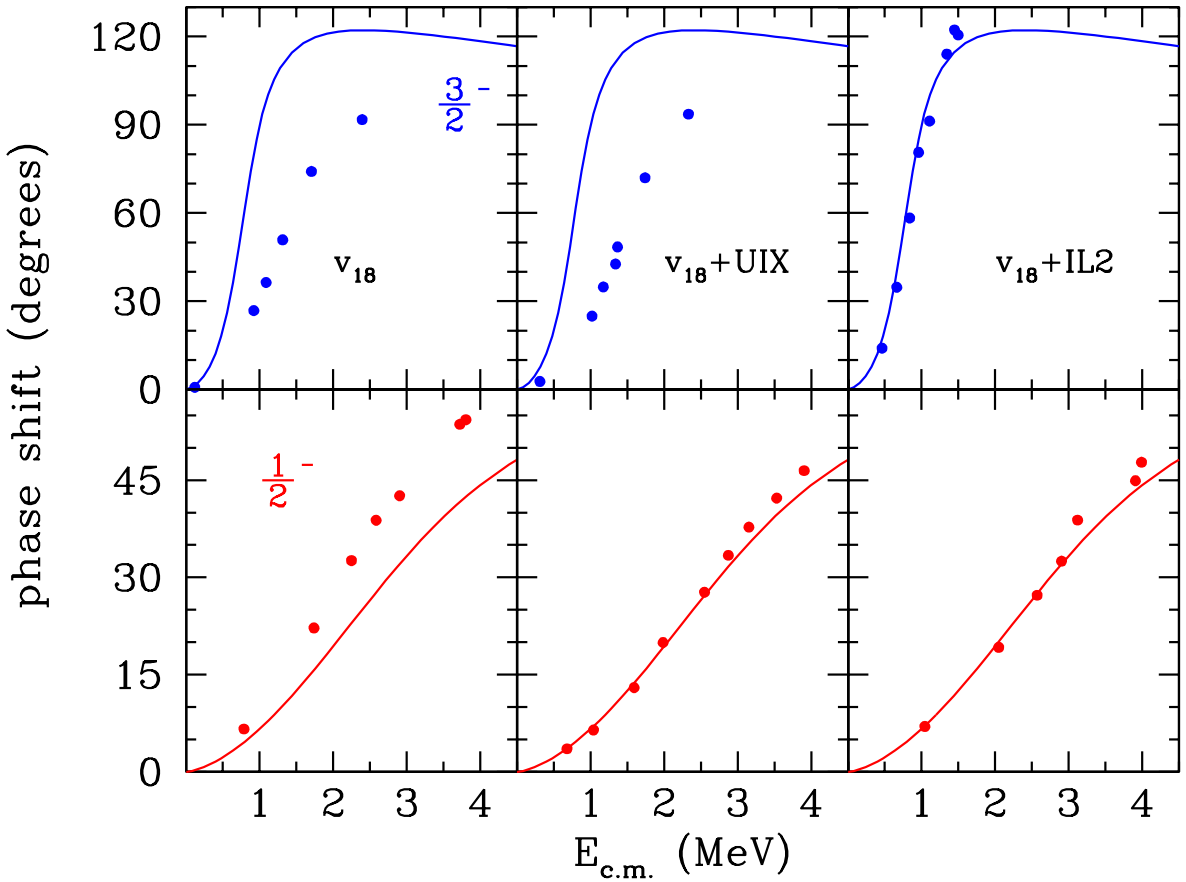
$$\Psi \propto \frac{1}{kr_{12}} \{\Phi_{c1}\Phi_{c2}Y_L\}_J \left[F_L(kr_{12}) \cos\delta_{JL} + G_L(kr_{12}) \sin\delta_{JL}\right] ,$$

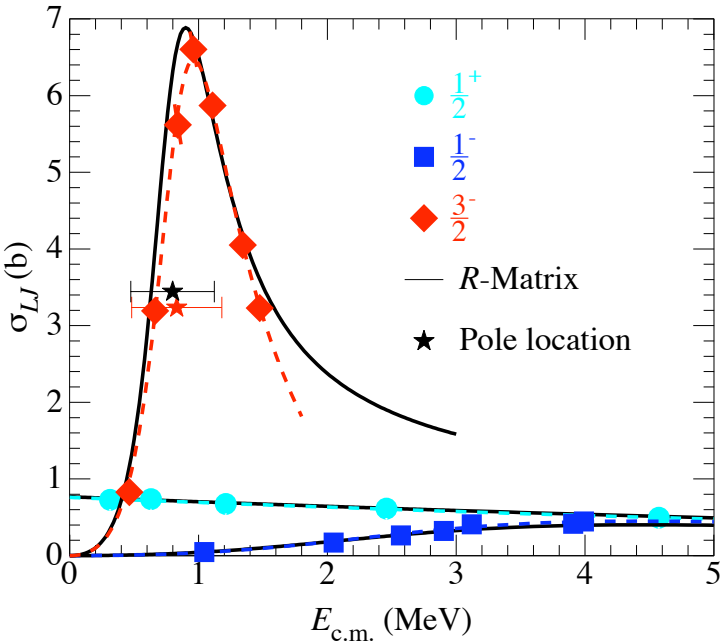
at the box surface

Scanning over boundary conditions γ maps out $\delta_{JL}(E)$

GFMC scattering: $^4\mathrm{He} + n$

We've done one complete GFMC scattering calculation, in ^{5}He
It linked splitting between $J^\pi = 3/2^-$ and $1/2^-$ states to 3-body force
(Backwards graphs: Fitted data are curves, points are GFMC)





Nollett et al. (2007)

Extracted S-matrix poles & scattering length are in good agreement with experiment

QMC scattering: Lessons learned

Building boundary & clusterization (near the boundary) into VMC is easy

GFMC is slow to asymptote in outer, noninteracting-cluster, parts of the box

Small inaccuracies in E calculation can cause headaches in matched δ_{JL}

Coupled channels (e.g. s- & d-waves of same J) will be a lot more work (preliminary $^3\mathrm{H} + n$ exists)

Isospin rotation of ^{5}He gave reasonable preliminary calculations of low-E ^{5}Li

Going to higher energies will require computing many states in the box (not just ground state at each γ), or finding a way to abandon the eigenvalue approach

The small remaining work to do n spin rotation is to choose γ at threshold & normalize the wave functions for unit flux

Extending NCSM with the resonating group method

In the 1970s & 1980s, the resonating group method (RGM) was developed for calculations of continuum states

You sort the nucleons into clusters (very simple single-configuration shell models)

A variational principle gives you Schrödinger-like coupled equations

$$\sum_j \mathcal{H}_{ij}\psi_j(r_{12}) = E\sum_j \mathcal{N}_{ij}\psi_j(r_{12})$$

At each E, which you solve for relative motion $\psi_i(r_{12})$ in each cluster channel i

Computation was more limited in the past decades: simple clusters & simple interaction (central & exchange terms, maybe $\mathbf{L}\cdot\mathbf{S}$, no tensor)

Merging RGM with NCSM

Navratil, Quaglioni, & collaborators have absorbed this formalism into NCSM

Instead of single-reference Hartree-like clusters, the clusters are full NCSM wave functions

The Hamiltonian comes from a realistic interaction (SRG-evolved)

Most of the computation goes into the "norm kernel" $\mathcal{N}_{ij}$, computed from antisymmetrized cluster products $\Phi_1\Phi_2$

With R-matrix boundary conditions at some surface & a discrete basis, continuum solution amounts to a matrix inversion

This builds in clusterization & lets you specify the E you want

NCSM/RGM or NCSMC: The fine print

In principle, there need to be many channels, including ones with all possible excitations of the clusters & types of rearrangements

In practice, that seems to be taken care of now by including an ordinary A-body NCSM wave function in the (overcomplete) basis

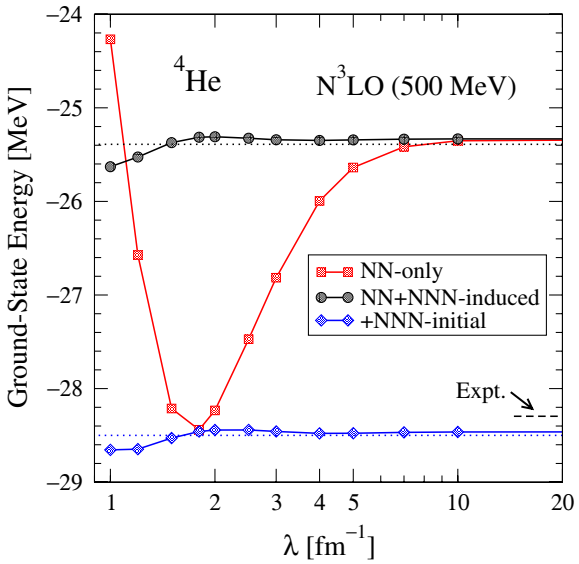
The purely NCSM version was "NCSM/RGM"

The hybrid approach is new (ca. 2013) & is called "NCSMC" (C for "continuum")

3-body interactions are still missing from a lot (but not all) of these calculations

It turns out you can tune the SRG evolution so that induced & bare NNN terms nearly cancel in E (works in s- & lower p-shell)

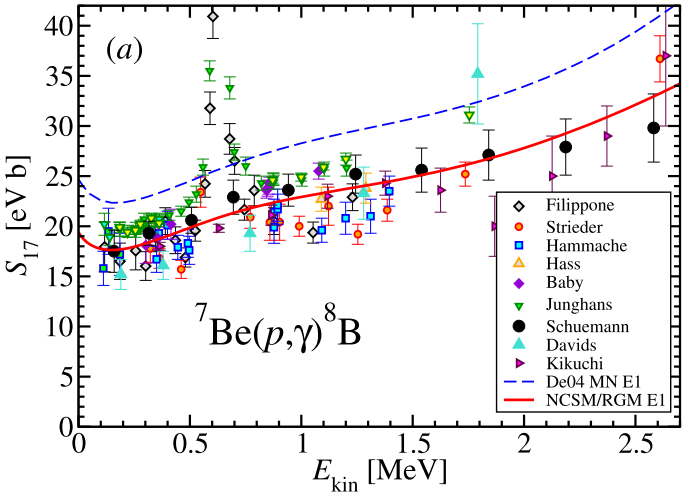
The "magic" SRG parameter value is $\lambda \sim 2.0$ fm^{-1}

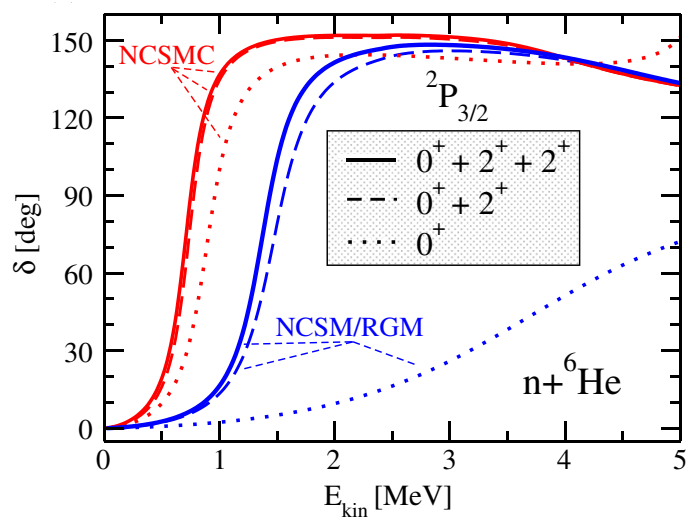


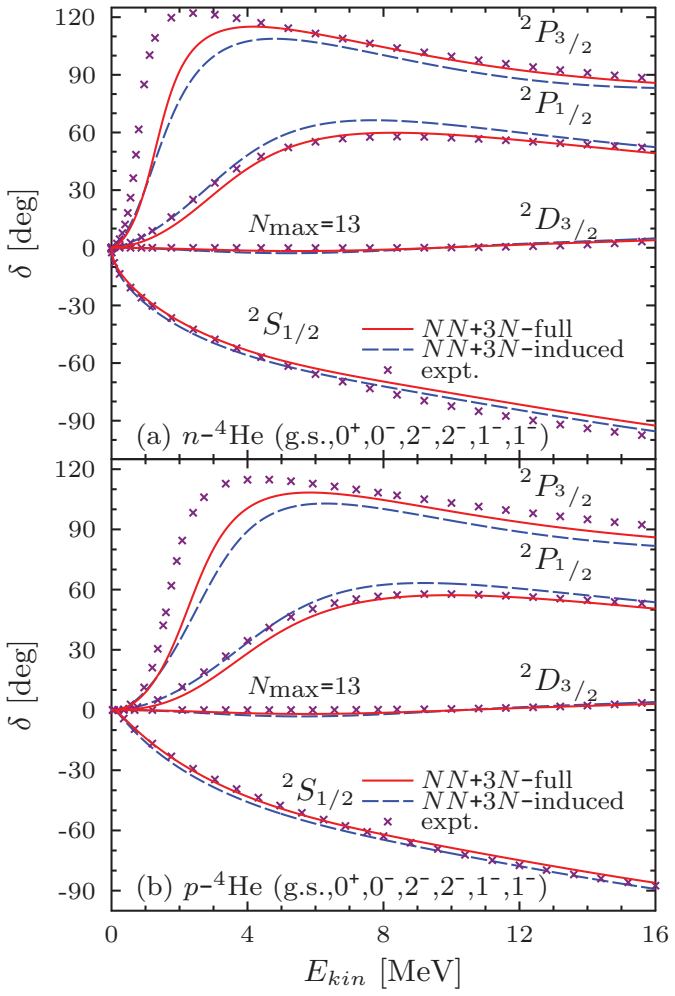
NCSM/RGM & NCSMC results

The results have been fairly impressive, first with no NNN, then magic λ, & now $A = 5$ with real NNN

I'll say more about radiative captures in a minute



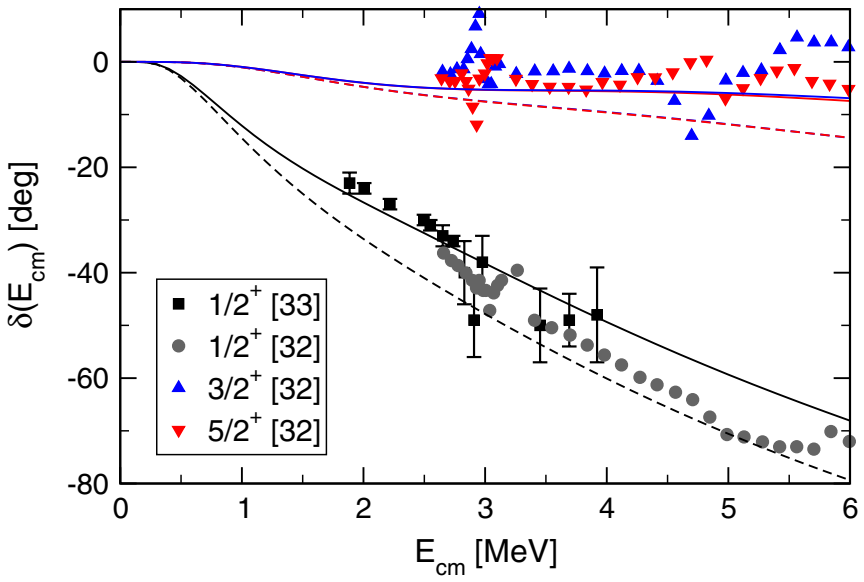


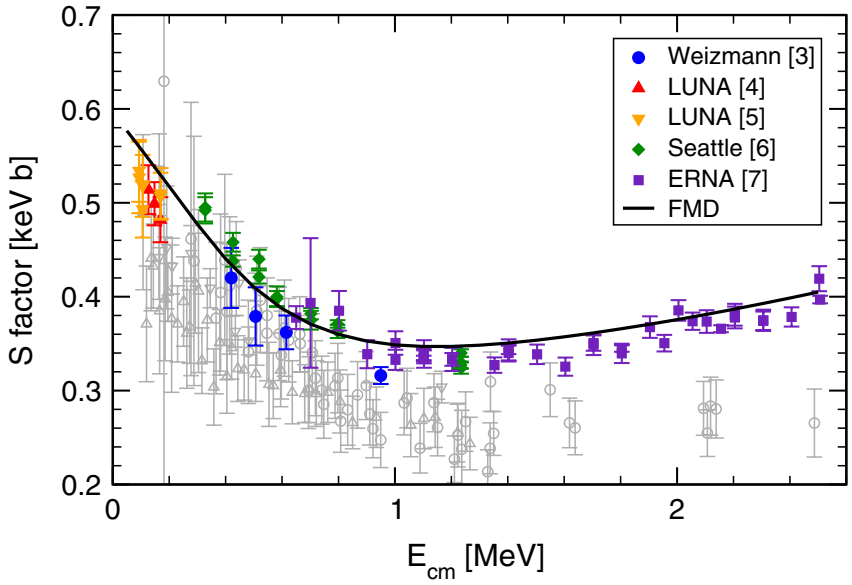


Still more efforts

There's been one scattering calculation using CC in a Gamow (complex-energy) basis ($^{40}\mathrm{Ca} + p$; Hagen & Michel 2012)

There has been a calculation of α capture in $^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$ & $^{3}\mathrm{H}(\alpha,\gamma)^{7}\mathrm{Li}$ by Neff (2011) with FMD





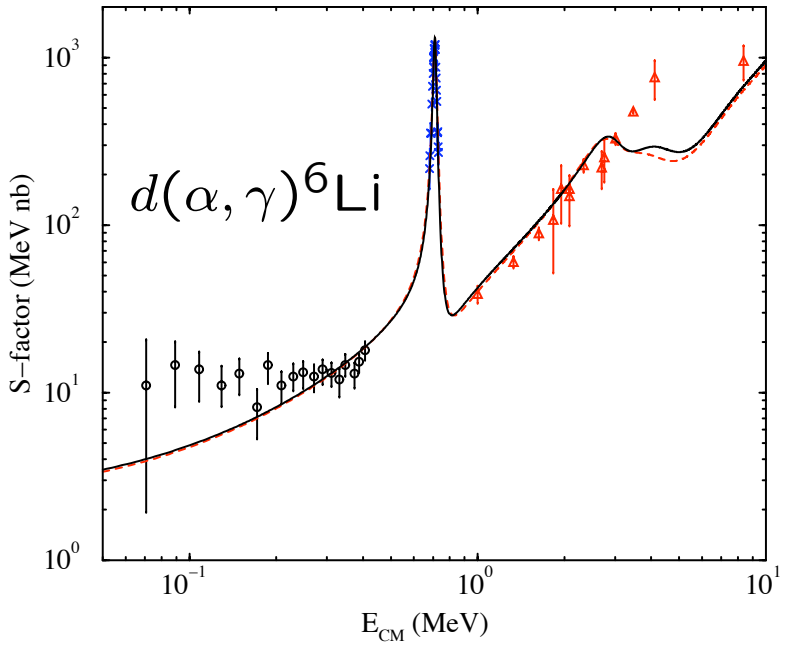
Something about $^{4}\mathrm{He}$ being spin-0 made this possible, so it may be a one-off

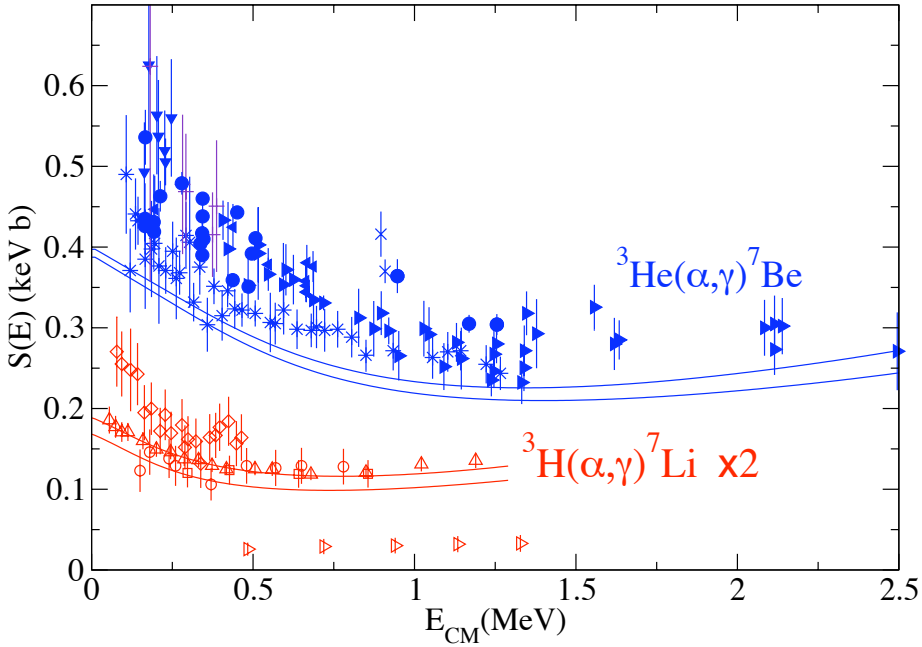
Semi-*ab initio* methods

Depending on available information & what you want, you might be better off "cheating" and mixing empirical & *ab initio* methods

I've done this a couple of times

Long ago (with Wiringa & Schiavilla, 2001), I computed α-captures with *ab initio* (VMC) clusters & final state but cluster motion from measured phase shifts

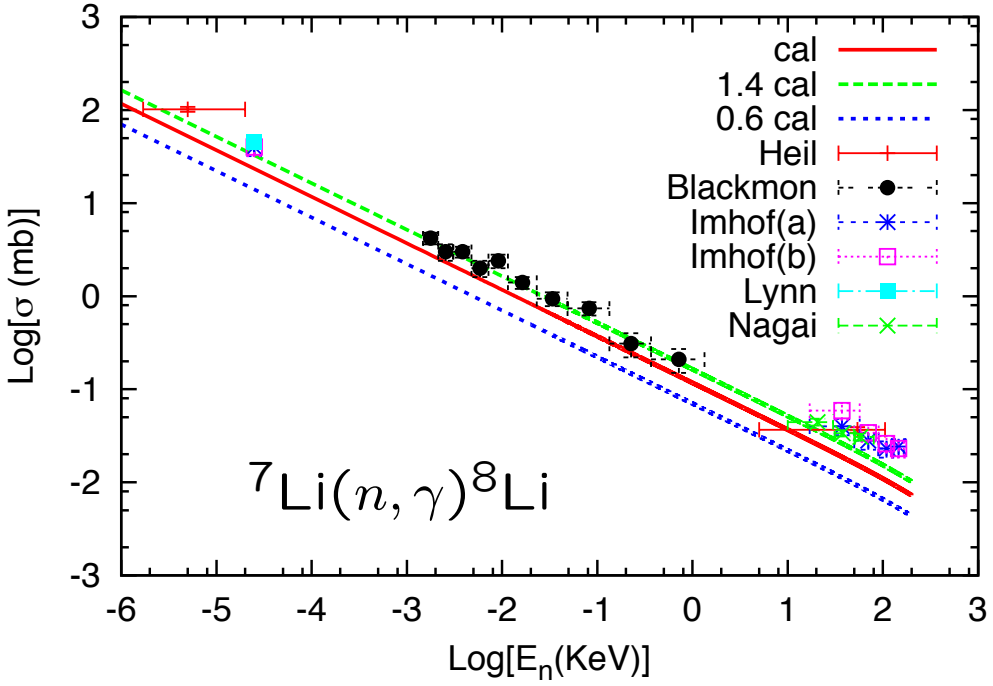


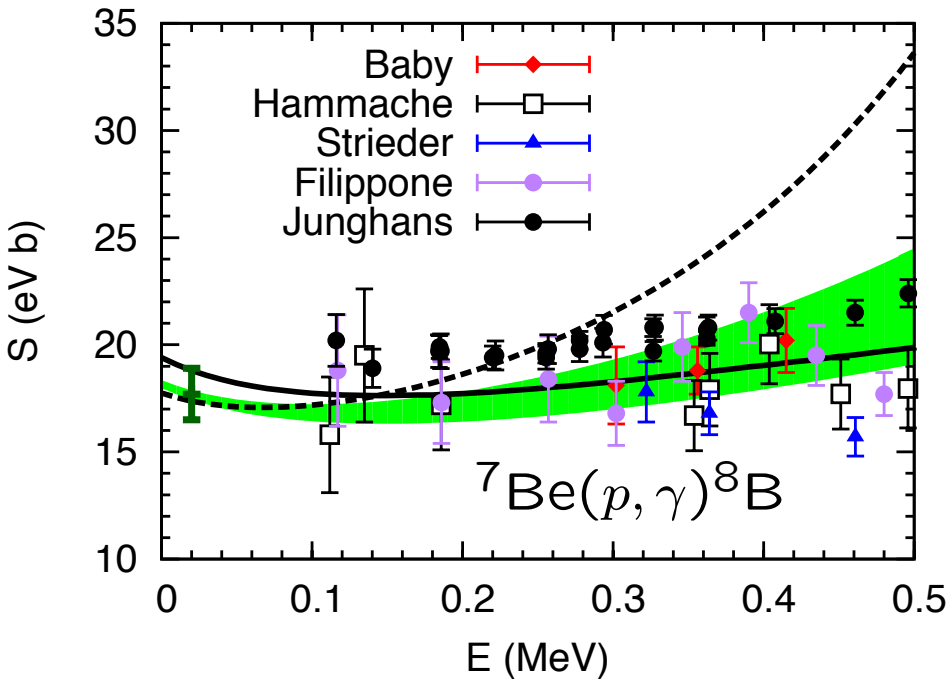


Ab initio inputs to halo EFT

If you want to produce the best cross section for some application, you'll want some nearly-consistent way of blending *ab initio* & empirical information

With this in mind, Zhang, Phillips & I have been working on halo EFT with mixed *ab initio* & empirical inputs (asymptotic normalizations & scattering lengths)





Some final thoughts on perturbative operators

Reaction observables that don't require a coupled-channel calculation are the easiest (at least for QMC)

For example:

Parity-violating $n\alpha$ spin rotation requires completely separate s- & p-wave calculations, then Fermi's golden rule with a PV operator

But $^3\mathrm{He}(n,p)^3\mathrm{H}$ requires coupling of $^3\mathrm{He}+n$ & $^3\mathrm{H}+p$ channels even without parity violation

The coupled channels can be dealt with, but more easily in some methods than others – the Pisa group has already dealt well with $^3\mathrm{He}(n,p)^3\mathrm{H}$ in the CHH basis

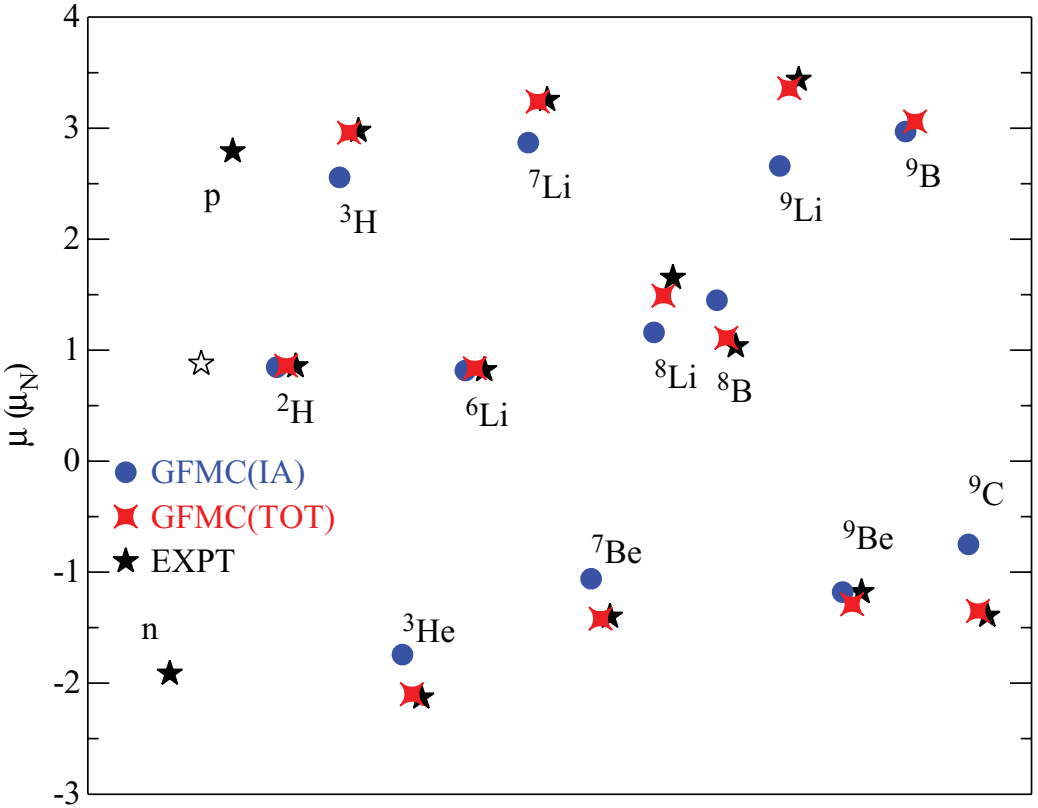
Lots of useful work was done with old-fashioned construction of current operators consistent with unevenly systematic NN potentials

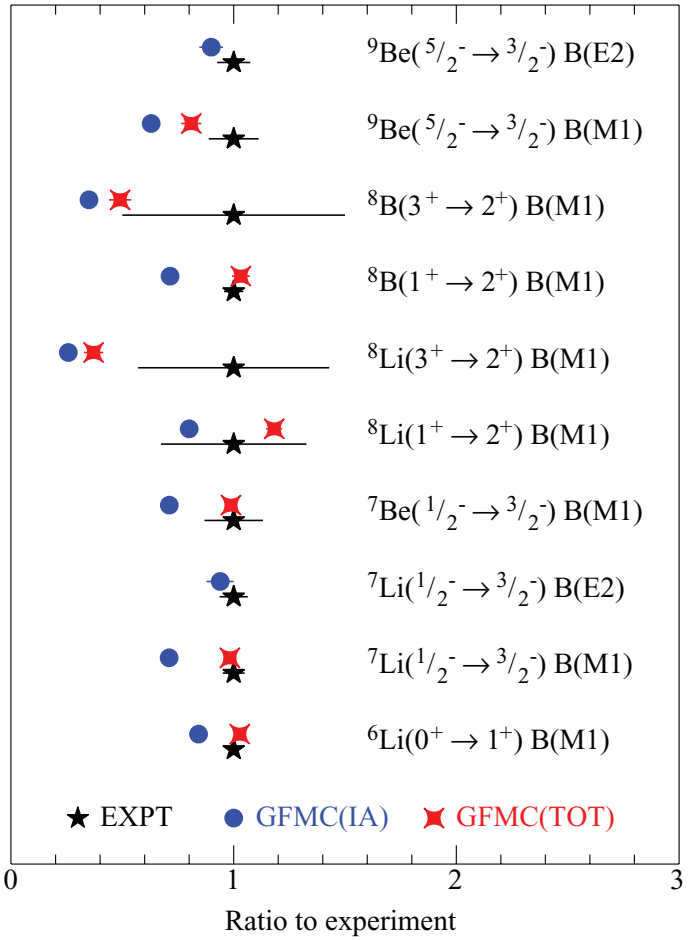
What you can do with good operators

Setting up operators in a consistent χEFT formalism with the NN interaction will avoid ambiguities & mismatches

Just using operators (including 2-body) from χEFT but matched for use with Argonne potential does quite well (mag. moments & transition strengths)

(From Pastore et al.)





Final final thoughts on operators

Putting some effort into consistency of perturbative operators & main NN force pays off with good reproduction of data

Fully consistent calculations are within reach

This requires currents (or symmetry-violating terms) established in a consistent formalism with the NN interaction

It also requires currents that are SRG-evolved in the same way as the NN potential (when that's done) – this is easily done now

More work is needed on currents consistent with truncated bases (e.g., how to get r.m.s. radius even in harmonic oscillator basis)

Final thoughts on *ab initio* continuum states

The unification of nuclear structure & reactions is widely recognized as important

There remain big mismatches between bound-state methods (e.g. VMC) & the reaction theory (e.g. DWBA) used to compare their results with experiment

Some difficulties remain in fixing 3-body interaction terms, but they can probably be dodged in many practical calculations

In light nuclei, few or no important features need to be fudged for percent-level precision in many observables

This field remains severely man- and womanpower-limited

BONUS MATERIAL