# Nuclear Structure and ISOL Facilities

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# Low-Energy Nuclear Physics Research

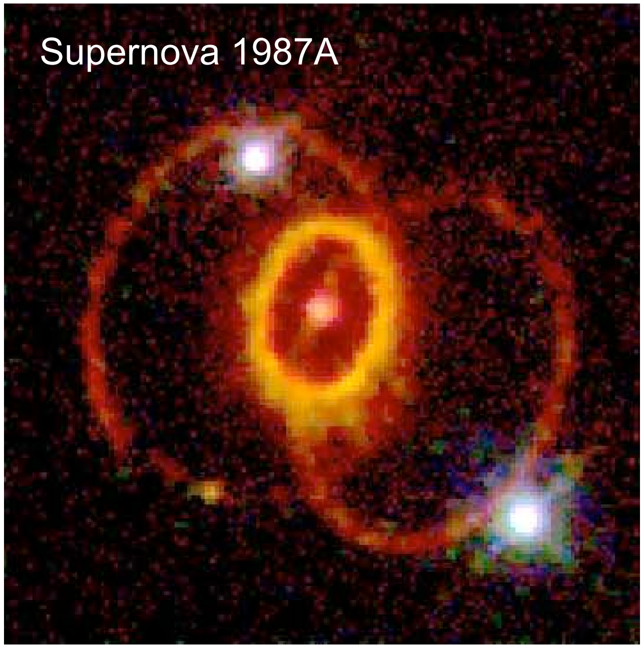
- Overarching goal:

**To arrive at a comprehensive and unified microscopic description of all nuclei and their low-energy reactions from the basic interactions between the constituent protons and neutrons**

- This is a lofty and ambitious goal that has been a "Holy Grail" in physics for over fifty years
- "Unified" does not mean that there is a single theoretical method that will work in all cases
  - Self-bound, two-component quantum many-fermion system
  - Complicated interaction with at least two- and three-nucleon components
  - We seek to describe the properties of "nuclei" ranging from the deuteron to super-heavy nuclei and neutron stars
- Symbiosis between theory and experiment
  - Experiment without theory is just a collection of information
  - Theory without experiment is just playing around

# Nuclear physics and the fate of the Universe

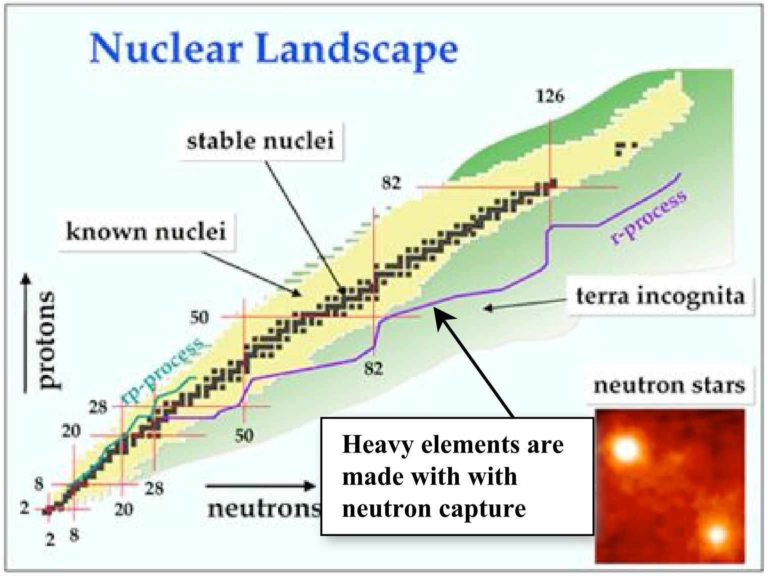
- Nuclear reactions are amongst the most important in the universe
  - They are responsible for all the matter we can see in the universe
- Big bang
  - Nothing much heavier than lithium
- Star formation
  - Fusion of light-ions can make elements up to Iron
  - Triple-alpha reaction to make $^{12}C$
- Supernovae (?)
  - Rapid neutron capture to make all elements up to Uranium




**"How were the elements from iron to uranium made?" -- one of the 'Eleven Science Questions for the New Century'** [*Connecting Quarks with the Cosmos*, Board on Physics and Astronomy, National Academies Press, 2003]

# Physics of exotic nuclei and the formation of the elements

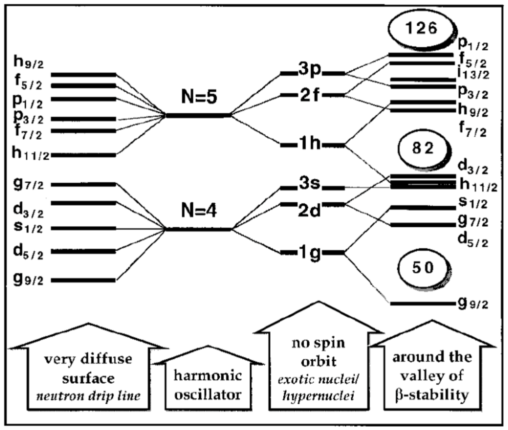
- Rapid neutron capture followed by beta decay to the valley of stability
- But much is unknown
  - Masses
  - Beta-decay lifetimes
  - Neutron capture rates
    - Density of states
    - Gamma strength functions
- Big question question
  - Where does the r-process occur?




**Nuclear properties are important in determining the fate of the universe**

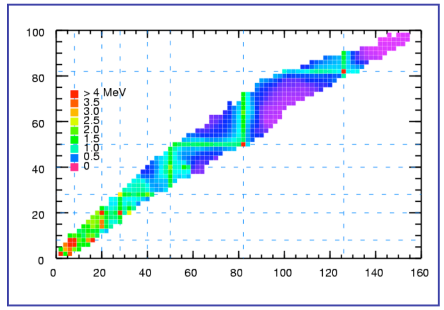
# The evolution of shell structure

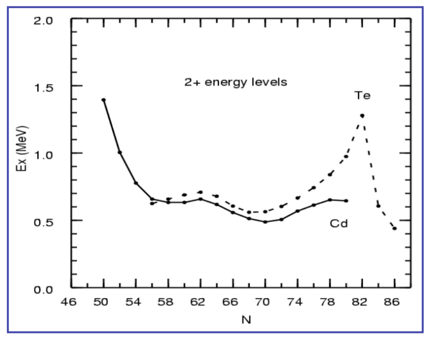
Our concept shell closures is probably not as universal as we once thought




Dobaczewski et al., PRC 53, 2809 (1996)

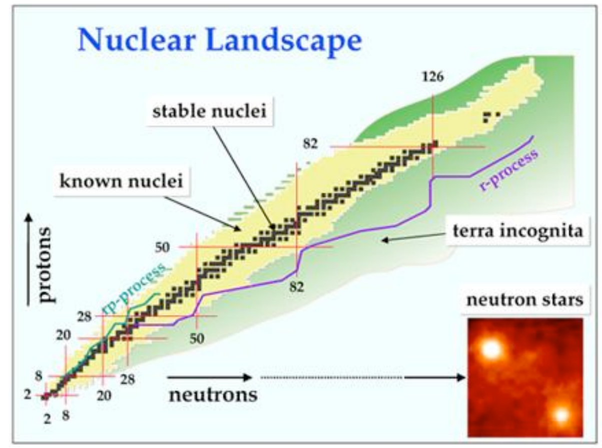
Experimental excitation energies for $2^+$ states

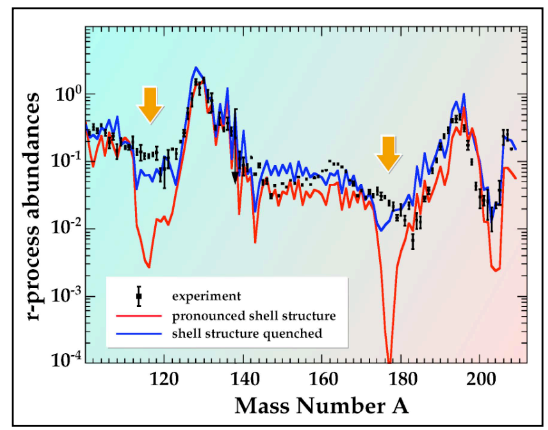



Dip at N=82, why?

Shell gaps and nucleosynthesis




**RIB facilities will help determine the properties of shell structures, but theory is essential.**

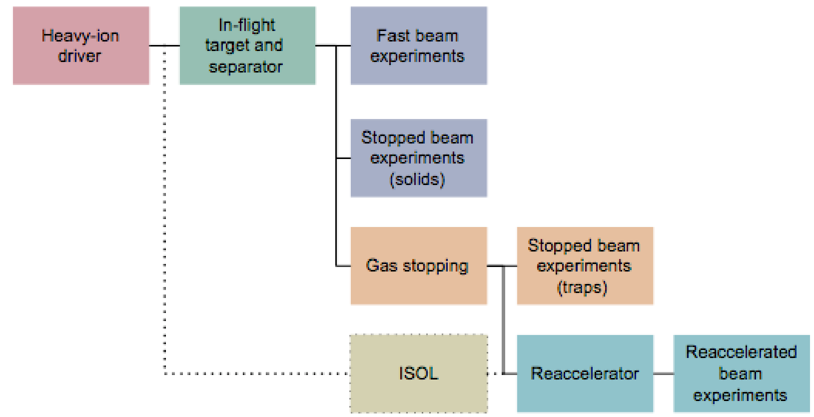
# What do we need?

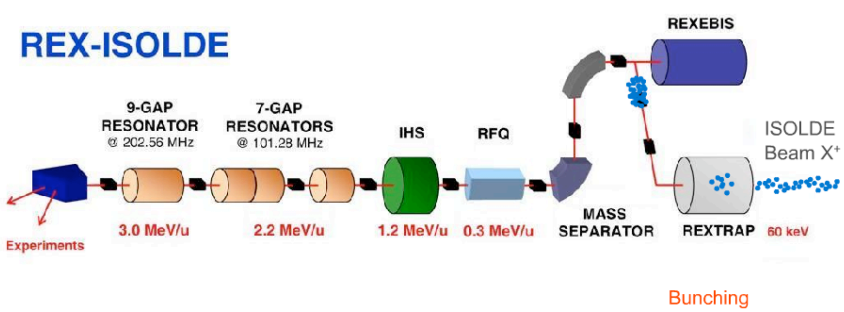
- More experimental data and better theories
  - Structure Theory
    - Masses
    - Beta-decay lifetimes
    - Level densities
    - Shell structures
  - Reaction Theory
    - Optical potential
    - Multi-step direct reactions theory
      - Break up
      - Surrogates
    - Pre-equilibrium emission

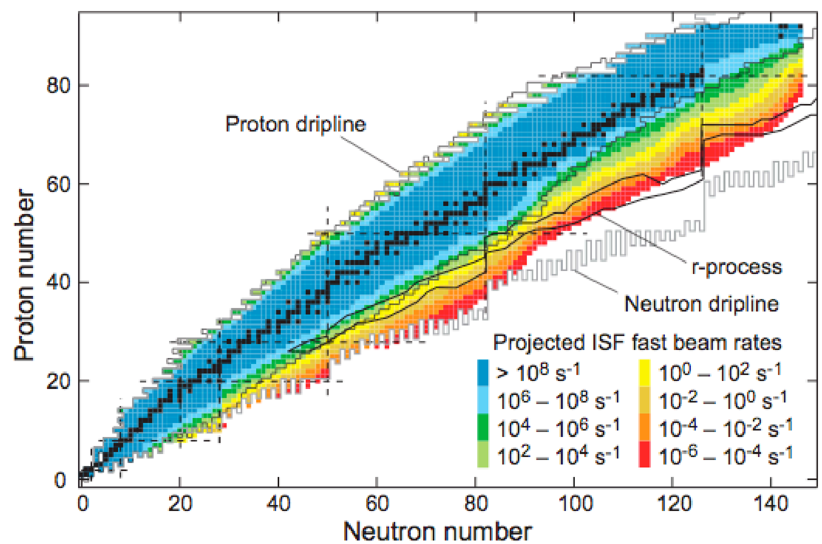
- Experiment can't do it all, and theory can't do it without experiment to validate the theories

# Tools of the future - Experiment

- New RIB facilities
  - RIKEN
  - GSI FAIR
  - EURISOL
  - GANIL
  - ISAC-TRIUMF
  - FRIB (aka RIA)
- Capabilities
  - Re-accelerated beams
  - Fast beams

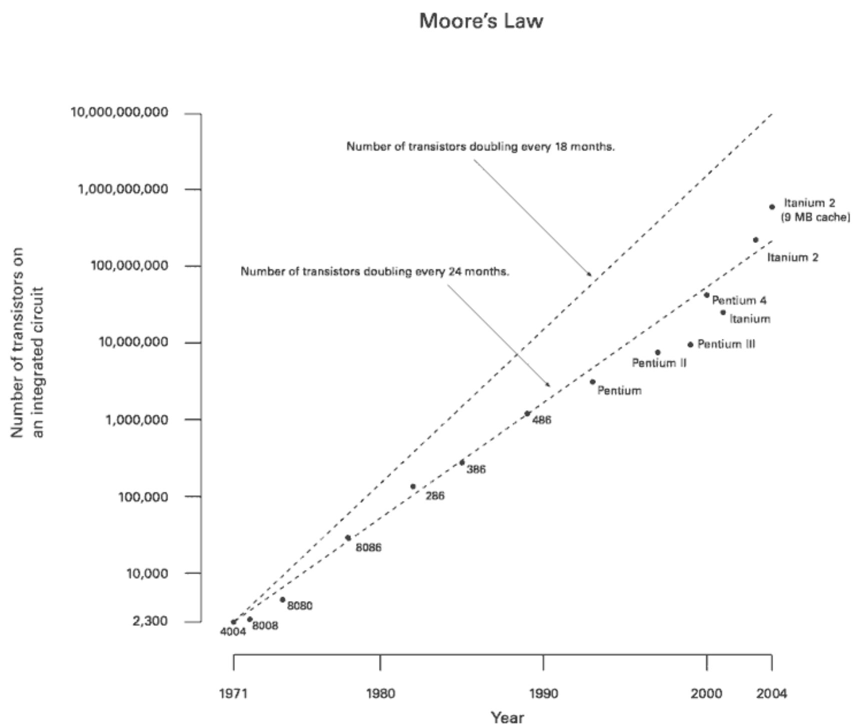


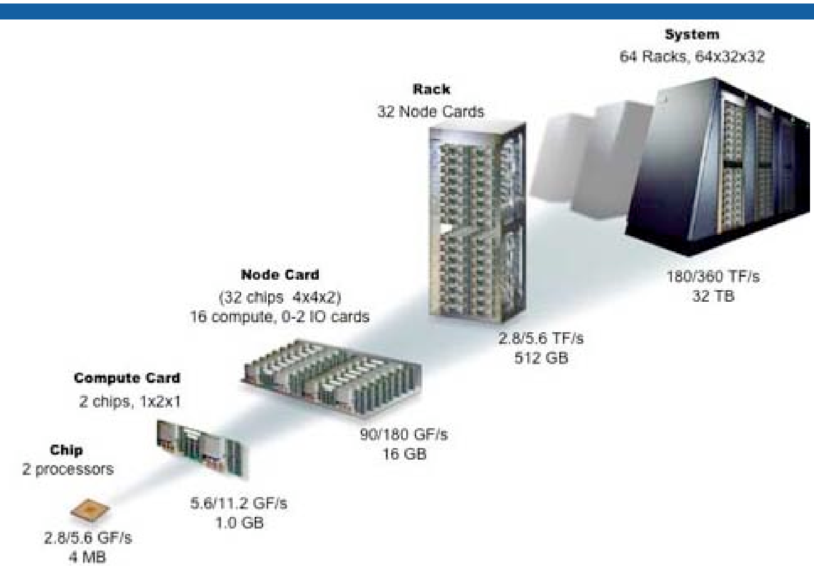



# Tools of the future - Theory

- Moore's law is a theorist's best friend

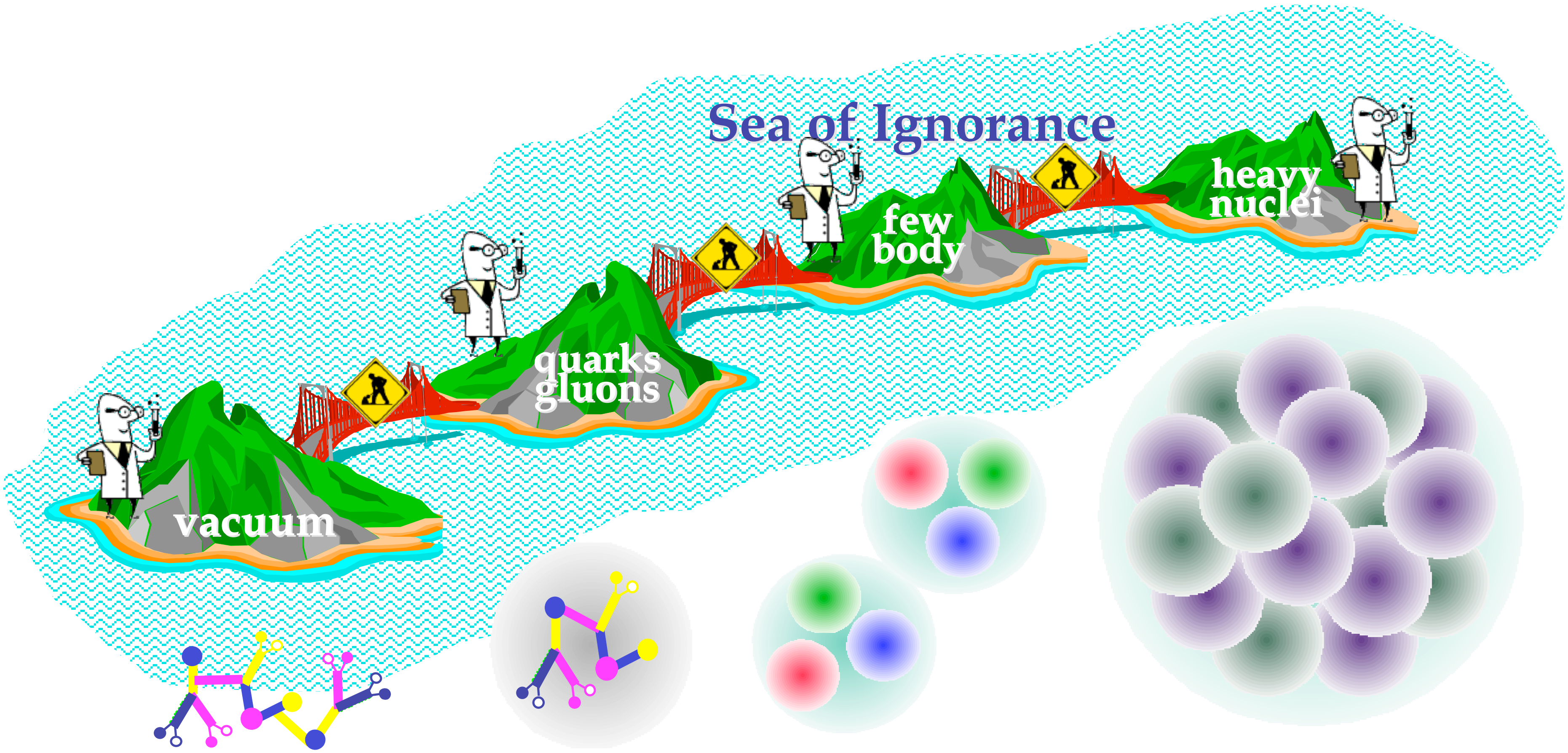



| Name | # Procs | Mem/proc | Tflops |
|---|---|---|---|
| BlueGene/L (1) | 65536 | 256MB | 367 |
| Purple (6) | 12288 | 4GB | 93 |
| Atlas (19) | 9216 | 2GB | 44 |
| Jaguar (2) | 23016 | 2GB | 119 |

**High-performance computing is giving us a tool that can revolutionize our approach to theoretical physics**

# Nuclear Many-Body Problem
# Energy, Density, Complexity




quark-gluon soup
QCD

nucleon
QCD

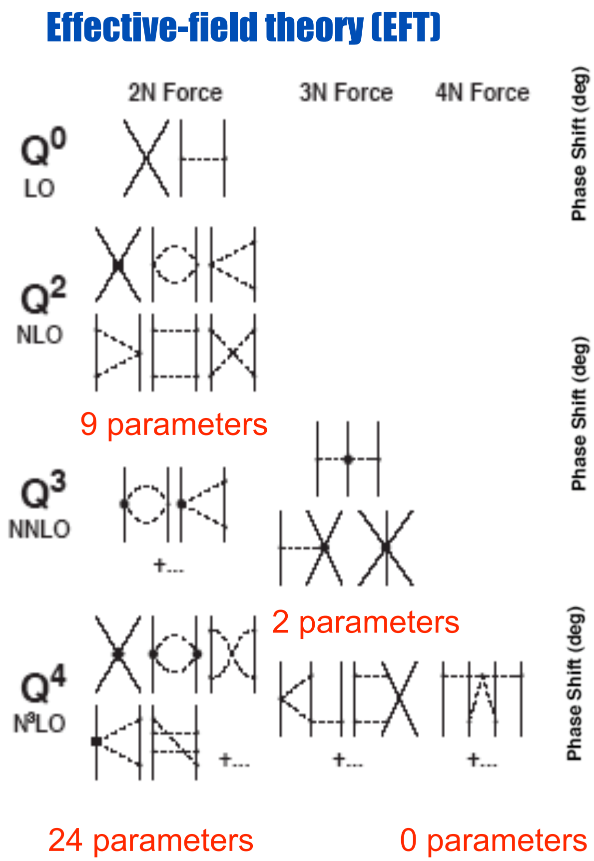
few body systems
free NN force

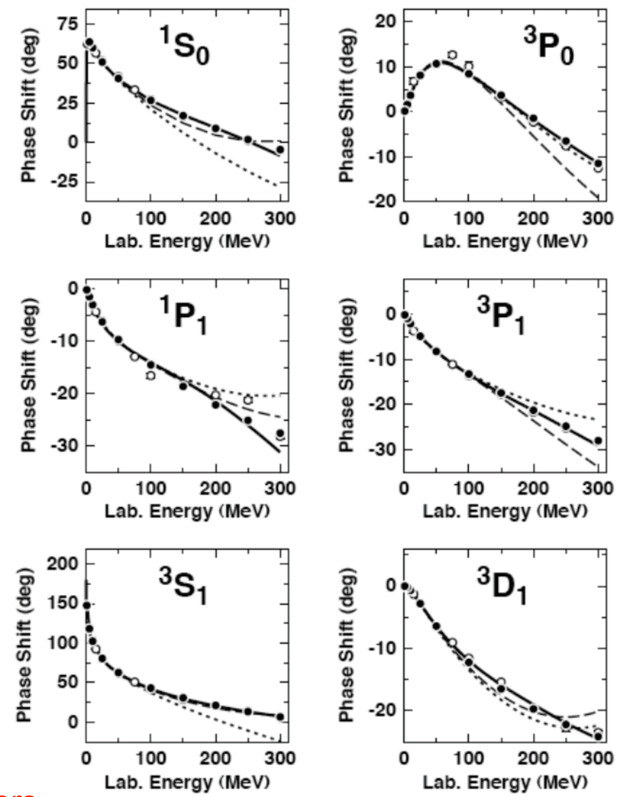
many body systems
effective NN force

# The Beginning - The Interaction

# The Beginning - The Interaction

- Inter-nucleon potentials
  - Paris, Argonne, Bonn, etc.
    - Potentials with parameters fit to scattering and bound state data
  - Effective-field theory
    - Guided by QCD with pion exchange with parameters fit to data
    - Order-parameter, $(Q/\Lambda)^n$ - $N^nLO$
  - $V_{low\text{-}k}$

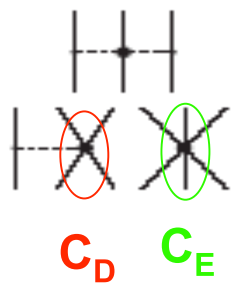


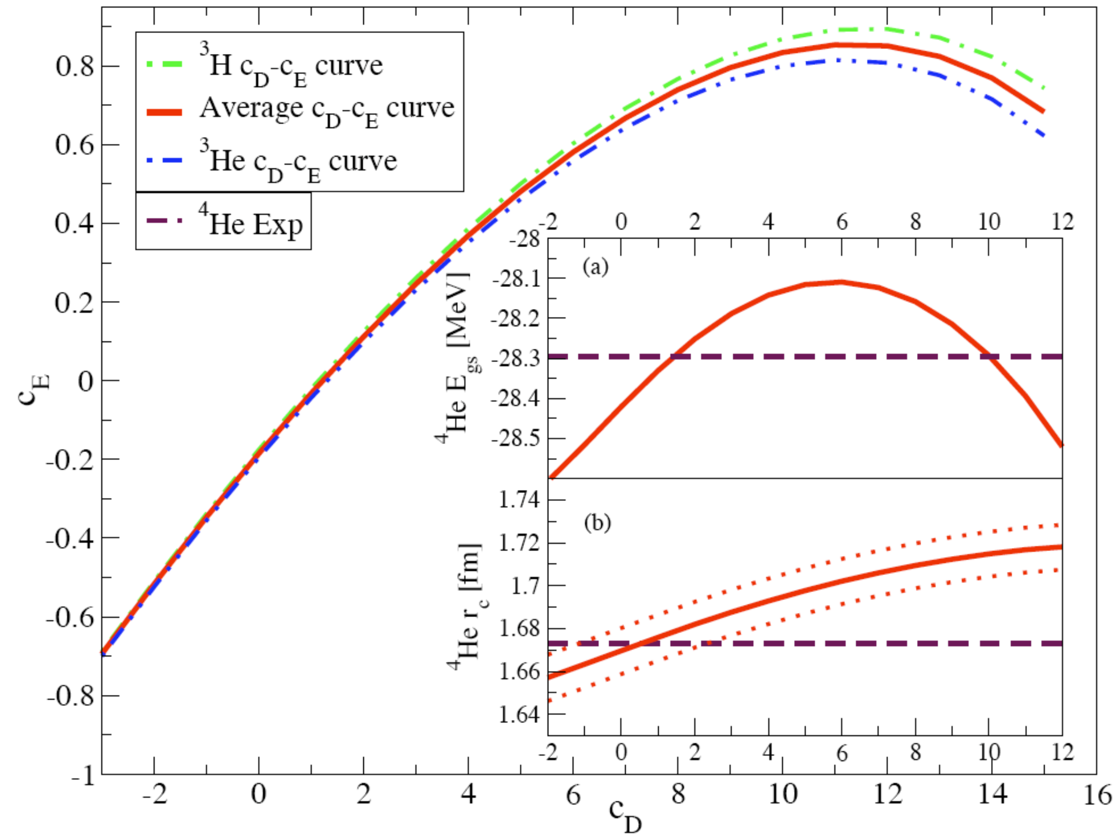

**EFT- two-body $N^3LO$, $\chi^2/\nu$ ~ 1: Entem et al., PRC68, 041001 (2003)**

# The Beginning - The Three-body Interaction

**$N^2LO$ 3-body**




- Also Illinois potential
  - GFMC - S. Pieper & B. Wiringa
- Question:
  - Can it solve the $A_y$ puzzle?
  - Is the NNN interaction the origin of spin-orbit physics in nuclei?



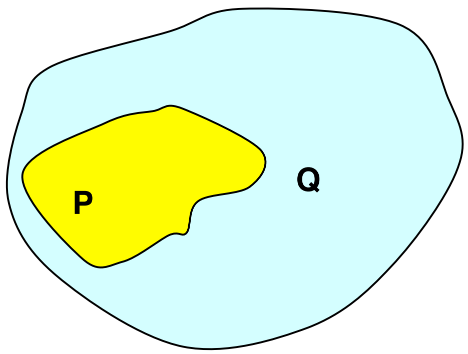

**Preference is $C_D \sim -1 - 0$**

**But, $C_D$ and $C_E$ are note well determined at $N^2LO$**

# Ab initio descriptions of light nuclei

# Can we get around this problem? Effective interactions

- Choose subspace of $\phi_n$ for a calculation (*P*-space)
  - Include most of the relevant physics
  - *Q* -space (excluded - infinite)




- Effective interaction:

$$H_{eff}\hat{P}\Psi_i = E_i\hat{P}\Psi_i$$

– Bloch-Horowitz

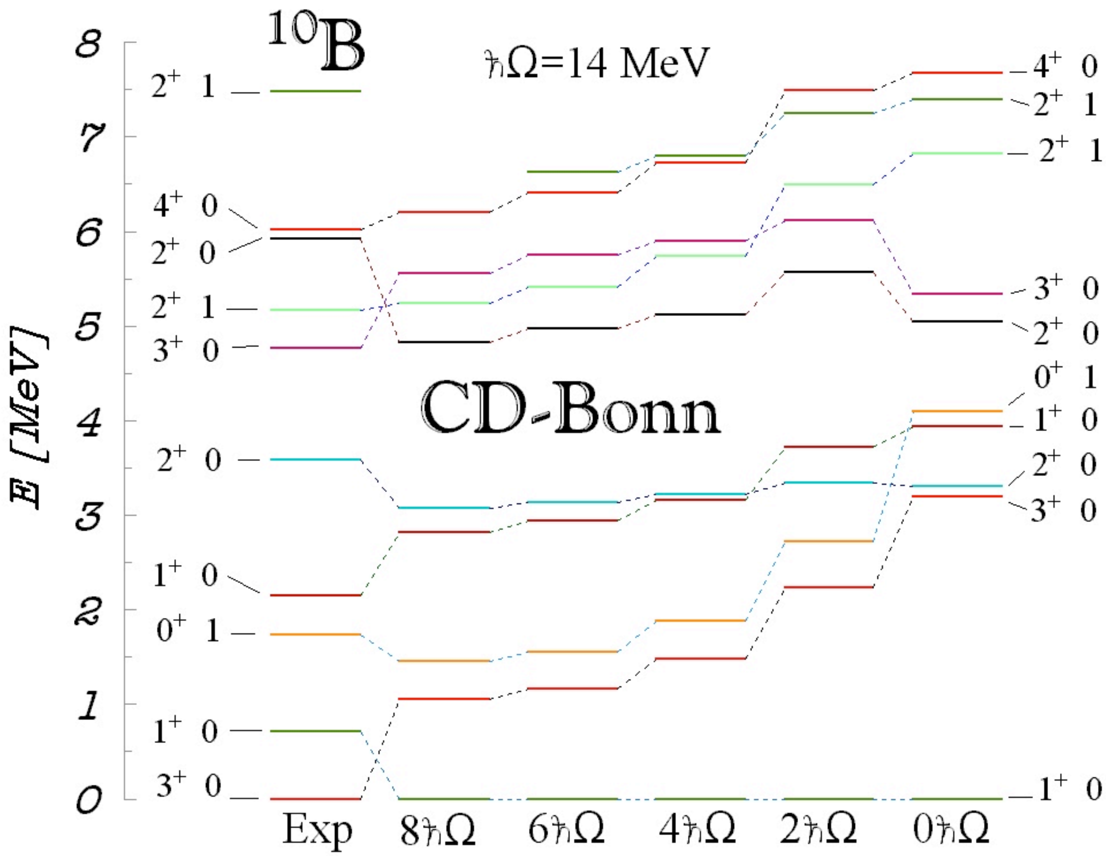
$$H_{eff} = \hat{P}H + \hat{P}H\frac{1}{E_i - \hat{Q}H}\hat{Q}H\hat{P}$$

– Lee-Suzuki:

$$H_{eff} = \mathbf{P}XHX^{-1}\mathbf{P}$$

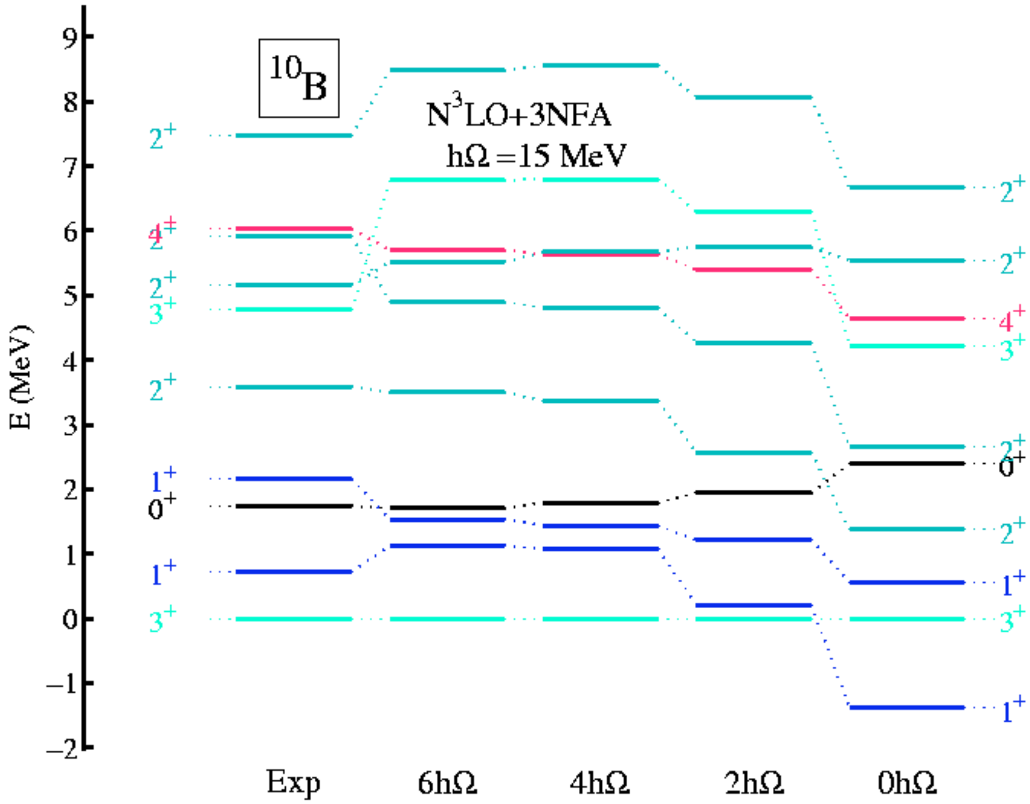
$$\mathbf{Q}XHX^{-1}\mathbf{P} = \mathbf{0}$$

# Deficiency of the NN interaction!




**$^{10}$B is one of the most important tests as all realistic NN-interactions fail to give the correct ground state**

# Three-body to the rescue




- Spin-orbit physics is coming from

- While the contact terms prevent collapse

Binding Energy (MeV)

Exp: -64.7507(3)

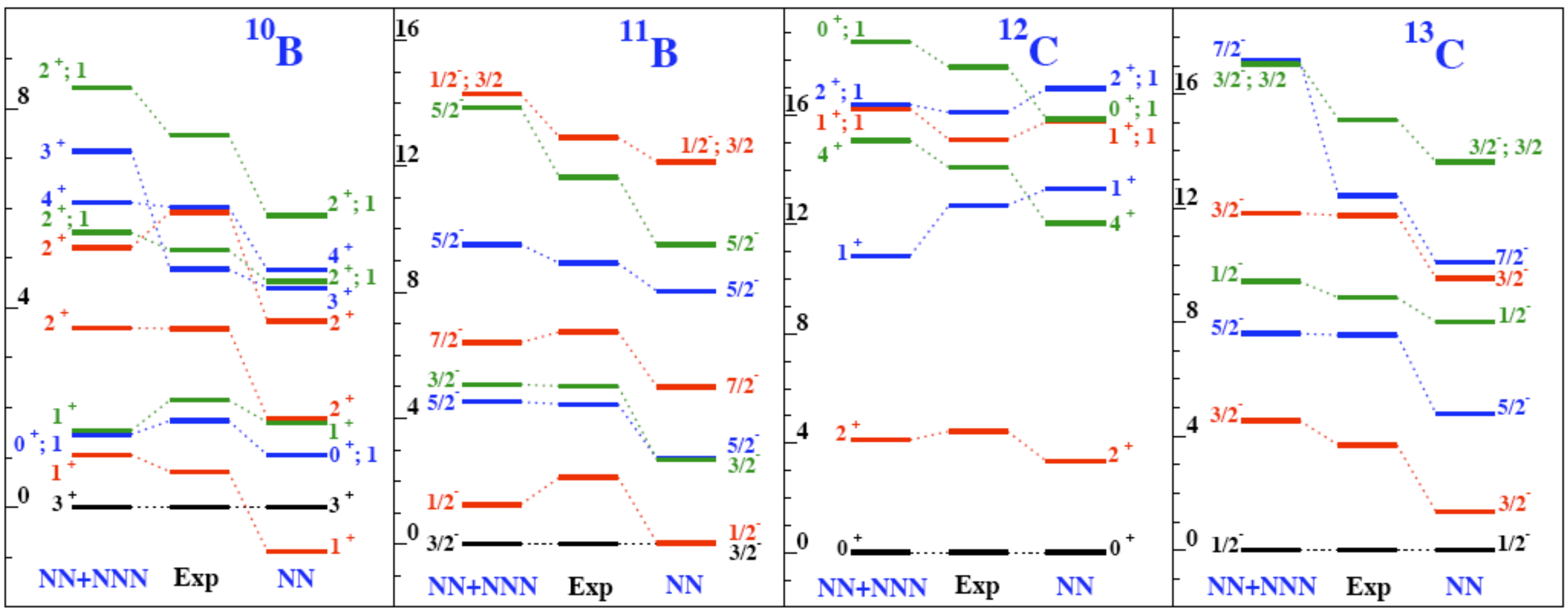
Thy: -64.03*

*Convergence study not completed

**Level ordering is in overall agreement with experiment.**
**$^{12}C$ to $^{16}O$ use ~ 6000 CPU hours with 3-body!**
**To be consistent we need to go to N³LO?**

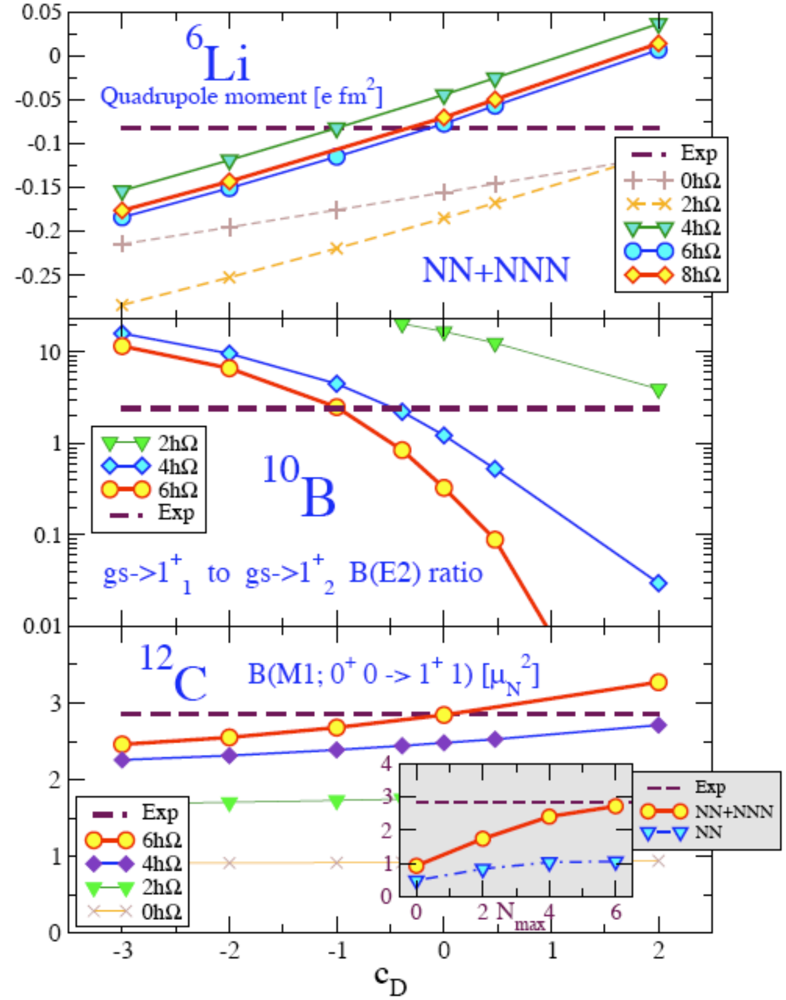
# The three-body interaction and level ordering

- No-core Shell Model (NCSM)
  - Oscillator basis $N_{\max}\hbar\Omega$
  - Effective interaction with Okubo-Lee-Suzuki transformation
  - Computationally challenging with three-body
    - $N_{max}$=6; $N_{basis}$~ 32M; 700M NNN m.e.; 6TB; 90TF; $N_{max}$=8 → 1.5 PF



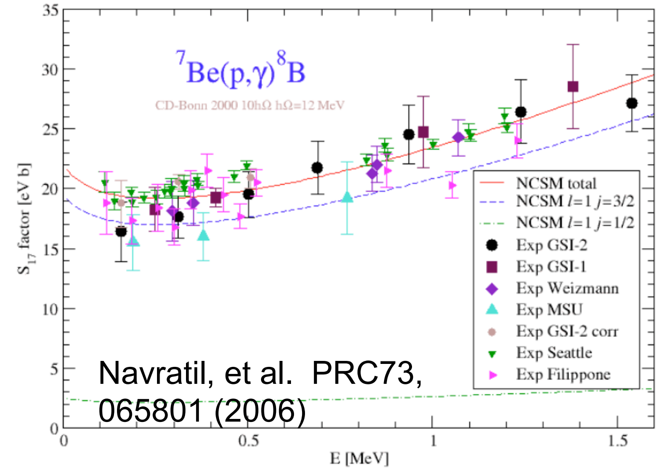
# The three-body interaction and transitions

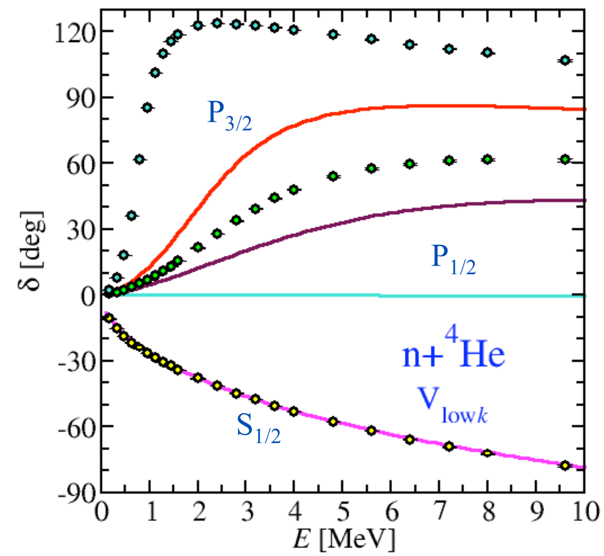
- M1 and Gamow-Teller are sensitive to the three-body interaction



# Reactions with the No-core Shell Model

- Light-ion fusion reactions
- First generation method
  - Not fully ab initio
  - Compute radial-cluster overlaps with NCSM
  - Woods-Saxon potential to fix asymptotic behavior and resonant state
- Resonating group method (RGM)
  - Fully ab initio

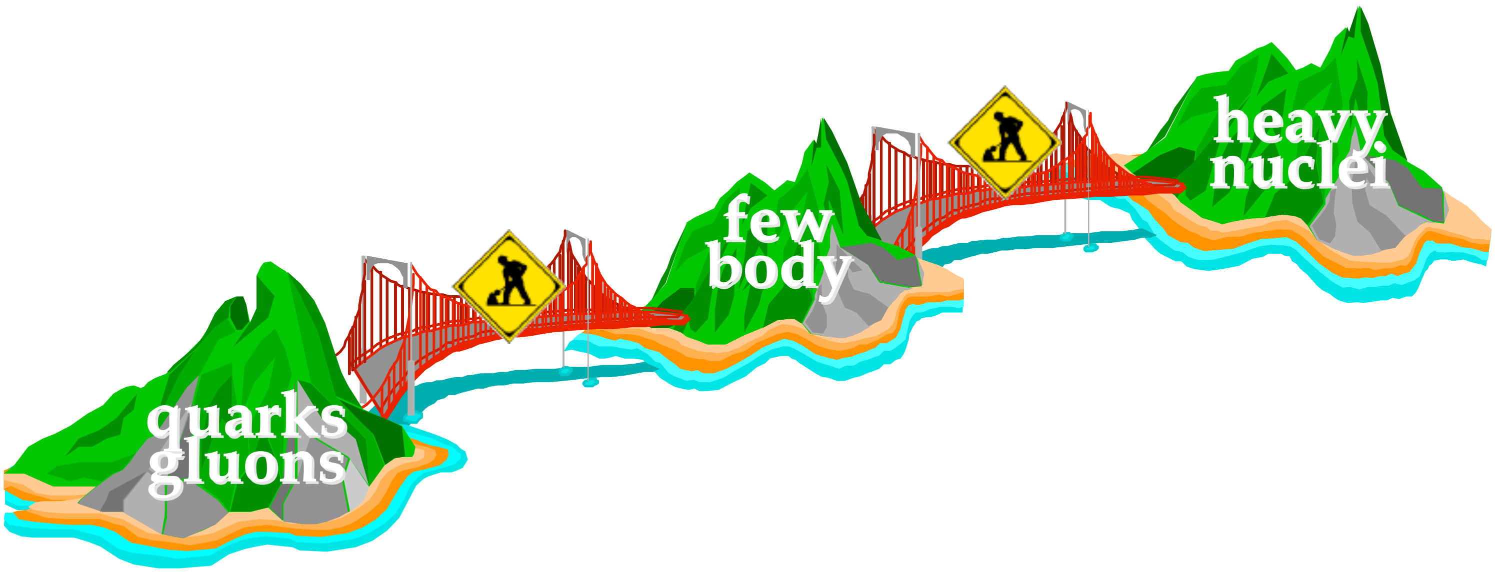


# Experiments to refine ab initio pictures

- Three-body interaction is poorly constrained
  - Masses and structure of drip-line nuclei are needed to help constrain the isospin structure of the three-body interaction
  - Gamow-Teller and M1 transitions to constrain the spin-orbit components of the three-nucleon interaction

# Beyond Light Nuclei



# Traditional methods suffer from computational overload

- Effective interaction needs to be derived!
  - No one really knows how to do this consistently today
- Large dimensions
  - Grows dramatically with number of particles
  - Consider half-filled fp-gsd

$$\mathrm{Dim} \approx \binom{N^p_{sps}}{n^p}\binom{N^n_{sps}}{n^n} \qquad \binom{50}{25}\binom{50}{25} = 1.9 \times 10^{28}$$

**Current computational capability of the order $10^{10}$ states**

**Even $10^{15}$ states would require a computer ~ $10^6$ times more powerful than any computer available today**

**$10^{20}$ IS NOT AN OPTION!**

# Auxiliary-Field Monte Carlo

- Try something different

**Thermal filter**

$$E_{GS} = \lim_{\beta\to\infty} \frac{\langle \psi_{trial} | e^{-\beta\hat{H}/2} \hat{H} e^{-\beta\hat{H}/2} | \psi_{trial} \rangle}{\langle \psi_{trial} | e^{-\beta\hat{H}} | \psi_{trial} \rangle}$$

**Thermal trace, T=1/β**

$$E(\beta) = \frac{Tr\left[\hat{H} e^{-\beta\hat{H}}\right]}{Tr\left[e^{-\beta\hat{H}}\right]}$$

- The Hamiltonian is two-body and the exponential $e^{-\frac{1}{2}\beta\sum_\alpha V_\alpha \hat{O}_\alpha^2}$ is impossible to deal with, so try

$$\int d\sigma_\alpha e^{-\frac{1}{2}\beta V_\alpha \left(\hat{O}_\alpha - s\sigma_\alpha\right)^2} = \sqrt{\frac{2\pi}{\beta|V_\alpha|}} \quad \rightarrow \quad e^{-\beta V_\alpha \hat{O}_\alpha^2} = \sqrt{\frac{\beta|V_\alpha|}{2\pi}} \int d\sigma_\alpha e^{-\beta|V_\alpha|\sigma_\alpha^2 + 2\beta s\sigma_\alpha V_\alpha \hat{O}_\alpha}$$

One-body operator

Gaussian factor

  - Two-body transformed to one-body - VERY GOOD
  - Introduced integral over an auxiliary field $\sigma$
    - These $\sigma$ fields have a physical meaning - think Hartree-Fock
    - Many $\sigma$ fields, also $e^{-\beta\hat{H}} \rightarrow \underbrace{e^{-\Delta\beta\hat{H}} \cdots e^{-\Delta\beta\hat{H}}}_{N_t \text{ time slices}}$

# Path integral formulation

$$e^{-\frac{1}{2}\Delta\beta\hat{H}} = \prod_\alpha \sqrt{\frac{|V_\alpha|}{2\pi}} \int \prod_\alpha d\sigma_\alpha e^{-\frac{1}{2}\Delta\beta\sum_\alpha |V_\alpha| \sigma_\alpha^2} e^{-\Delta\beta\sum_\alpha (\varepsilon_\alpha - V_\alpha s_\alpha \sigma_\alpha)\hat{O}_\alpha}$$

- Transformed the many-body trace into a path integral and a trace over a one-body Hamiltonian

$$\langle \hat{O} \rangle = \frac{\int D(\vec{\sigma}) e^{-\frac{1}{2}\Delta\beta\sum_{\alpha,n} |V_\alpha| \sigma_{\alpha,n}^2} Tr\left[e^{-\Delta\beta\hat{h}(\sigma_{N_t})} \dots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right] \frac{Tr\left[\hat{O} e^{-\Delta\beta\hat{h}(\sigma_{N_t})} \dots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]}{Tr\left[e^{-\Delta\beta\hat{h}(\sigma_{N_t})} \dots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]}}{\int D(\vec{\sigma}) e^{-\frac{1}{2}\Delta\beta\sum_{\alpha,n} |V_\alpha| \sigma_{\alpha,n}^2} Tr\left[e^{-\Delta\beta\hat{h}(\vec{\sigma}_{N_t})} \dots e^{-\Delta\beta\hat{h}(\vec{\sigma}_{N_t})}\right]}$$

$$= \frac{\int D(\vec{\sigma}) W(\vec{\sigma}) \langle \hat{O} \rangle_{\vec{\sigma}}}{\int D(\vec{\sigma}) W(\vec{\sigma})}$$

# Auxiliary-Field Monte Carlo

- We now have a multi-dimensional (many thousands!) integral

$$\langle \hat{O} \rangle = \frac{Tr\left[\hat{O}e^{-\beta\hat{H}}\right]}{Tr\left[e^{-\beta\hat{H}}\right]} = \frac{\int D[\vec{\sigma}]W(\vec{\sigma})\langle \hat{O} \rangle_{\vec{\sigma}}}{\int D[\vec{\sigma}]W(\vec{\sigma})} \quad \rightarrow \quad \langle \hat{O} \rangle_{\mathrm{MC}} = \frac{1}{N}\sum_k \langle \hat{O} \rangle_{\vec{\sigma}_k \in W(\sigma)}$$

$10^{22}$ states → $2\times10^5$ fields

But W(σ) must be positive

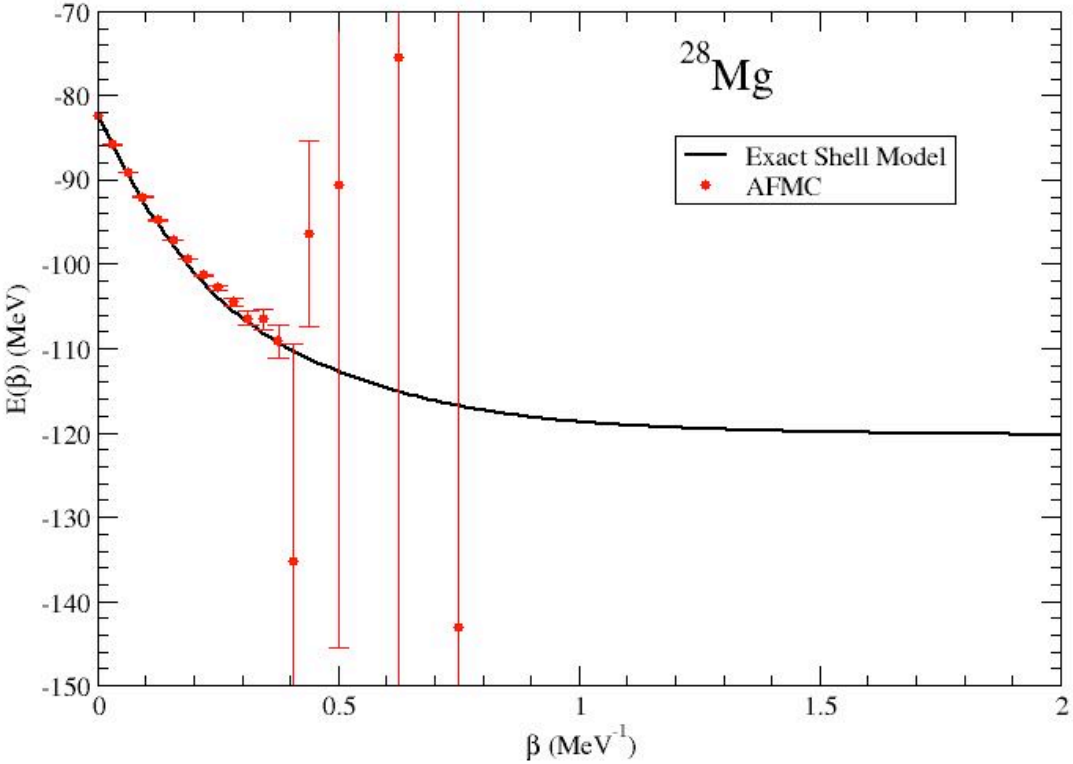
But, in general, W(σ) is not positive definite

$$\langle \hat{O} \rangle = \frac{\int D[\vec{\sigma}]\left|W(\vec{\sigma})\right|\langle \hat{O} \rangle_{\vec{\sigma}} W(\vec{\sigma})/\left|W(\vec{\sigma})\right|}{\int D[\vec{\sigma}]\left|W(\vec{\sigma})\right|W(\vec{\sigma})/\left|W(\vec{\sigma})\right|} \quad \rightarrow \quad \langle \hat{O} \rangle_{\mathrm{MC}} = \frac{\sum_k \langle \hat{O} \rangle_{\vec{\sigma}_k} W(\vec{\sigma}_k)/\left|W(\vec{\sigma}_k)\right|}{\sum_k W(\vec{\sigma}_k)/\left|W(\vec{\sigma}_k)\right|}$$

# The Sign-problem

- Problem: In general, W(σ) has bad sign

Thermal Energy for $^{28}Mg$

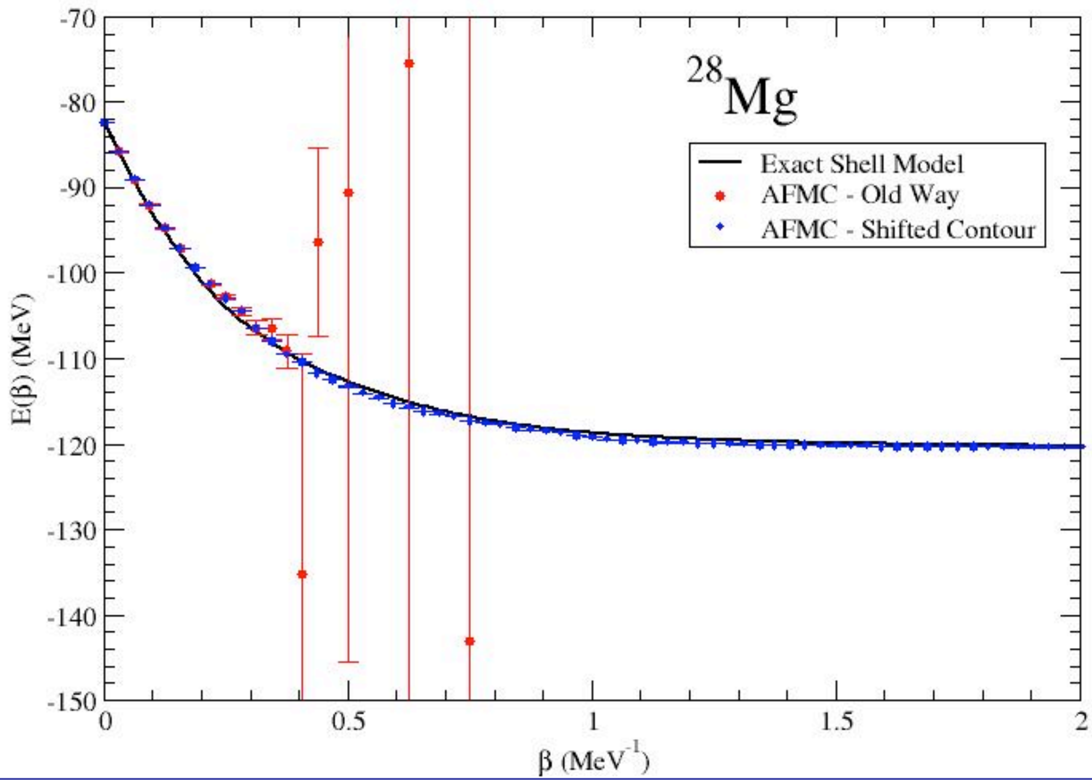



**AFMC was essentially useless for realistic interactions**

# Defeating the Sign Problem

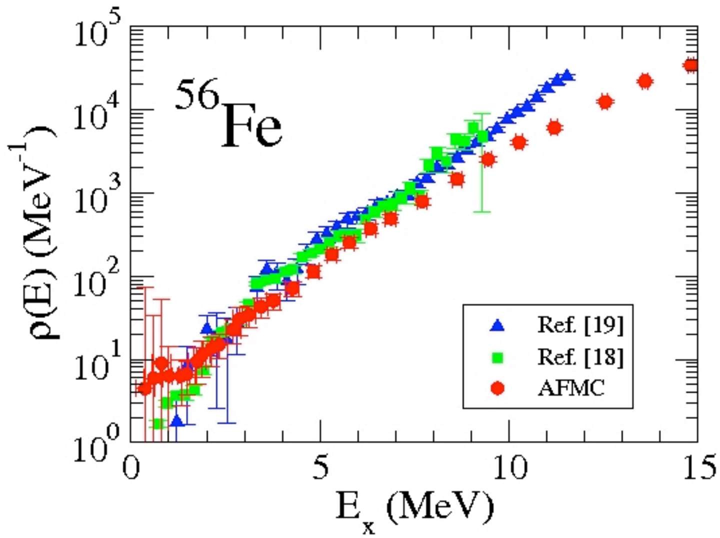
- Introduce a shift in the Hamiltonian [maximum of $W(\sigma)$]

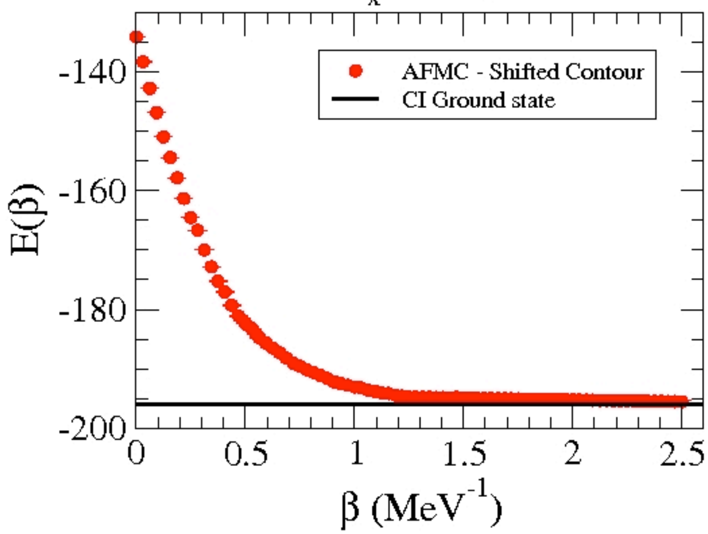
$$H = \sum_\alpha V_\alpha \left(\hat{O}_\alpha - \tilde{\sigma}_\alpha\right)^2 + 2V_\alpha \tilde{\sigma}_\alpha \hat{O}_\alpha - V_\alpha \tilde{\sigma}_\alpha^2$$




**First successful application with a realistic interaction**

# Results: $^{56}Fe$





18. A. Schiller *et al.*, Phys. Rev. C **68**, 054326 (2003).
19. A. V. Voinov *et al.*, Phys. Rev. C **74**, 014314 (2006).


$$E_{CI} = -195.901 \qquad \approx 1000 \text{ CPU hr}$$

$$E_{AFMC} = -195.687(107) \qquad \approx 12 \text{ CPU hr}$$

**We can solve the general CI problem exactly**

# Summary

- Incredible progress over the past five years
- The Future looks bright!
  - Link between QCD and NN, NNN, and NNNN interactions
  - *Ab initio* solutions for light nuclei - A ~ 20
  - Methods are being developed to treat heavy nuclei
  - Theory coupled with experiment will expand our understanding of nuclei
    - New RIB facilities
    - High-performance computing