# From QCD to the nuclear many-body problem: theory and experiments at Isolde

Morten Hjorth-Jensen

Department of Physics and Center of Mathematics for Applications
University of Oslo, N-0316 Oslo, Norway

[2]Department of Physics and Astronomy, Michigan State University
East Lansing, Michigan, USA

May 12, 2009

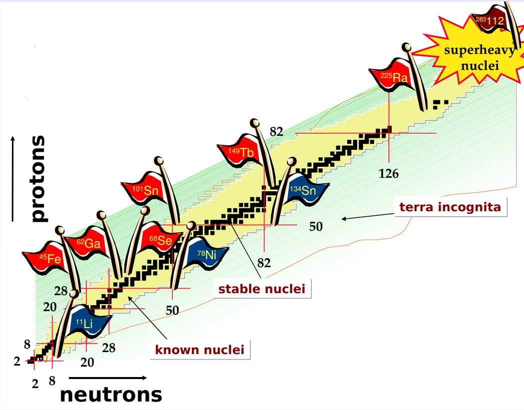
# Outline

1. Introduction
2. Theory status and perspectives
3. Theory and experiment, why HIE-Isolde?
4. Summary and perspectives

# Two take-away messages

**Large advances in recent years**

- Nuclear scientists, experimentalists and theorists, are getting better and better at controlling short-lived nuclei, in particular those which are useful
- Rare isotopes are the key to answering questions in many areas of science and HIE-isolde will play an important role



# Further observations

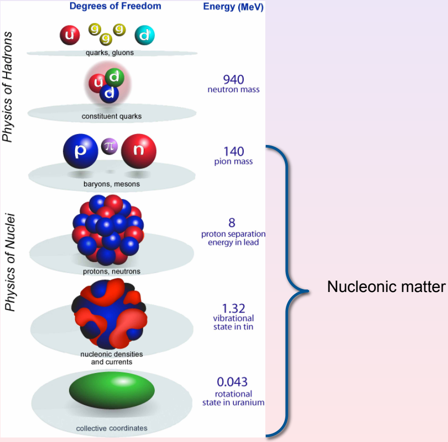
## From OECD Global Science Forum, Nuclear Physics Working Group

- Basic nuclear physics research as conducted today is very international in nature. The community has identified 90 user facilities in 26 countries, with the largest concentration in Europe, Japan and the USA. There is a wide diversity in the size, complexity and costs of the facilities needed, which include accelerators, reactors and underground laboratories.
- **Major advances are occurring in theoretical studies of nuclear systems. Algorithmic and computational advances hold promise for breakthroughs in predictive power, enhancing the strong links between theory and experiment. For a number of specific topics, interdisciplinary collaborations have developed which have been very successful.**

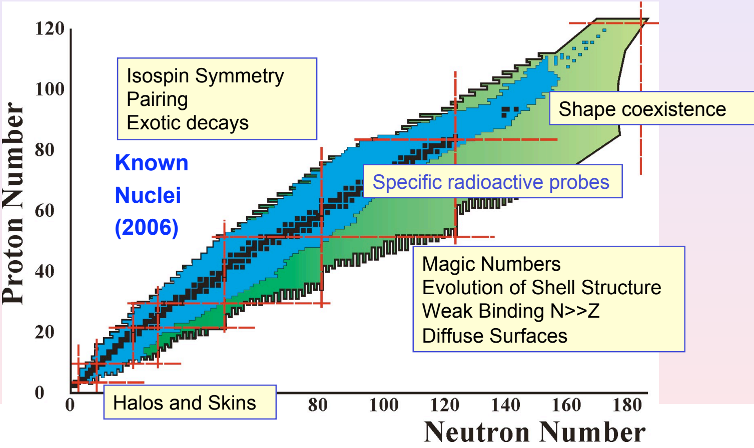
# Important questions from QCD to the nuclear many-body problem

- How to derive the in medium nucleon-nucleon interaction from basic principles?
- How does the nuclear force depend on the proton-to-neutron ratio?
- What are the limits for the existence of nuclei?
- How can collective phenomena be explained from individual motion?
- Shape transitions in nuclei?

The many scales pose a severe challenge to *ab initio* descriptions of nuclear systems.



# Mapping some of the previous questions on the chart of nuclei



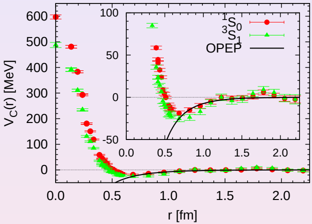
# Aims, motivations and challenges

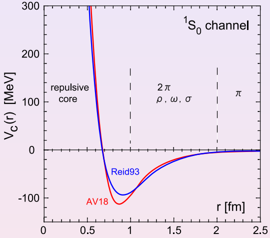
1. Facilities like HIE-Isolde which address the physics of radioactive ion beams can offer unprecedented data on weakly bound systems and stability of matter.
2. Crucial for Nuclear physics next 10-15 years : understand how shells evolve and how matter is held together
3. Identify and investigate methods that will extend to unstable systems
4. Want an 'ab initio' and reductionist approach starting with a nuclear Hamiltonian constrained from effective field theory and QCD.
5. We see now a possible merging of effective field theories with ab initio many-body methods, great promise for a truly quantitative description of nuclei.
6. Want to marry many-body calculations calculations with reaction theory.

# Progress in our QCD understanding of the NN force

- Explore the limits of our understanding of the atomic nuclei based on nucleonic and mesonic degrees of freedom. CEBAF, J-Parc, FAIR and LHC offer such perspectives.
- Experimental plans aim at identifying and exploring the transition from the nucleon/meson description of nuclei to the underlying quark and gluon description.
- Test the short-range behavior of the NN interaction via deep inelastic scattering
- Effective field theory has made progress in constructing NN and NNN forces from the underlying symmetries of QCD
- Three-body and higher-body forces emerge naturally and have explicit expressions at every order in the chiral expansion.
- Recent progress in Lattice QCD (LQCD) may hold great promise for constraining effective field theories.
- LQCD will be able to tell us about the interactions of systems that cannot be probed experimentally, but have relevance to astrophysics (nucleon-hyperon interactions), meson-meson and meson-baryon interactions, and other fields of nuclear physics.

# Lattice QCD, Ishii *et al*, nucl-th/0611096, PRL 2007





Can we constrain the NN and NNN interactions from Lattice QCD? More likely to use Lattice QCD to constrain parameters in Effective field theory. Unrealistic pion masses used in the calculations. (hep/lat:0710.1827, hep/lat:0707.1670, hep/lat 0706.3026, hep/lat:0810.2331)

# Modeling of nuclear interactions

1. Meson-exchange theory of Yukawa (1935)
2. Fujita-Miyazawa three-nucleon potential (1955)
3. First phase-shift analysis of *NN* scattering data (1957)
4. Gammel-Thaler, Hamada-Johnston and Reid phenomenological potentials (1957–1968)
5. Bonn, Nijmegen and Paris field-theoretic models (1970s)
6. Tuscon-Melbourne and Urbana *NNN* potential models (late 70's–early 80's)
7. Nijmegen partial wave analysis (PWA93) with $\chi^2$/dof$\sim 1$ (1993)
8. Nijm I, Nijm II, Reid93, Argonne $v_{18}$ and CD-Bonn (1990s)
9. Effective field theory (EFT) at $N^3LO$ (2004–)
10. Can we constrain parameters in EFT from lattice QCD? In the mesonic sector, constraining EFT parameters from LQCD has been definitely demonstrated. With petascale and soon exascale, this will happen in the baryonic sector as well!

# Status of 2N and 3N Interactions from Effective Field Theory

Nucleons and Pions as effective degrees of freedom only. Chiral perturbation theory for different orders ($\nu$) of the expansion in terms of momentum/pion mass.

| Chiral order | 2N force | 3N force | 4N force |
|---|---|---|---|
| $\nu = 0$ | $V_{1\pi} + V_{\mathrm{cont}}$ | – | – |
| $\nu = 1$ | – | – | – |
| $\nu = 2$ | $V_{1\pi} + V_{2\pi} + V_{\mathrm{cont}}$ | – | – |
| $\nu = 3$ | $V_{1\pi} + V_{2\pi}$ | $V_{2\pi} + V_{1\pi,\,\mathrm{cont}} + V_{\mathrm{cont}}$ | – |
| $\nu = 4$ | $V_{1\pi} + V_{2\pi} + V_{3\pi} + V_{\mathrm{cont}}$ | work in progress | work in progress |

# Simulations, theory and experiment

## Theory

### Connections to computational science

1Teraflop=$10^{12}$ flops
1peta=$10^{15}$ flops (next 2-3 years)
1exa=$10^{18}$ flops (next 10 years)

http://www.top500.org/

**challenge: utilize leadership class computers**

**EXAMPLE:** ***SCIDAC 2***
***Universal Nuclear Energy Density Functional***

- Funded by
  - Office of Science
  - ASCR
  - NNSA
- 15 institutions
- ~50 researchers
  - physics
  - computer science
  - applied mathematics
- foreign collaborators

http://unedf.org/

**…unprecedented theoretical effort !**

# Nuclear Many-Body Methods

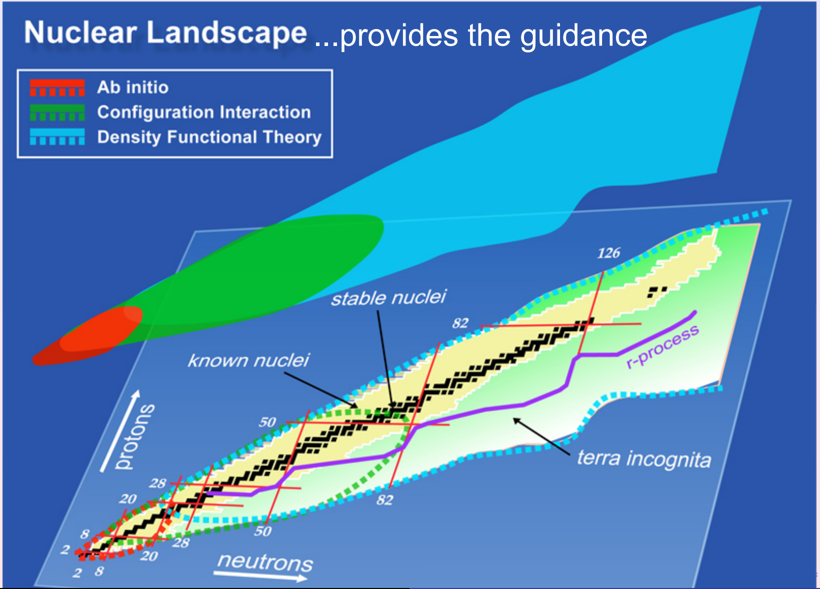
## Widely used Methods

1. Variational and Diffusion Monte Carlo/GFMC ($A \leq 12$)
2. Large-scale diagonalization methods, either few particle or few single-particle degrees of freedom
3. Coupled cluster theory, possibly all closed-shell nuclei
4. Perturbative many-body methods
5. Green's function methods, ab initio Density functional theory, etc..
6. Extentions to weakly bound systems, Gamow shell model, complex scaling, etc..

# Ab initio State of the Art

1. $^2$H by numerical integration (1952) – a pair of coupled second-order differential equations in 1 variable. At the time this took between 5 and 20 minutes for the calculation and the printout another 5 minutes!
2. $^3$H by Faddeev (1975–1985)
3. $^4$He by Green's function Monte Carlo (GFMC) (1988)
4. $A = 6 - 7$ by GFMC (1994-98)
5. $A = 8$ by GFMC and no-core-shell-model (NCSM) (2000)
6. $^4$He benchmark by 7 methods to 0.1% (2001-2008)
7. $A = 9, 10$ by GFMC and NCSM (2002)
8. $^{12}$C by GFMC and NCSM (2004–)
9. $A = 4, 16, 40, 48, 56$ by Coupled Cluster theory (CC) (2005–), tin within 2009
10. Chain of helium and oxygen isotopes by Coupled Cluster (2007-2009)

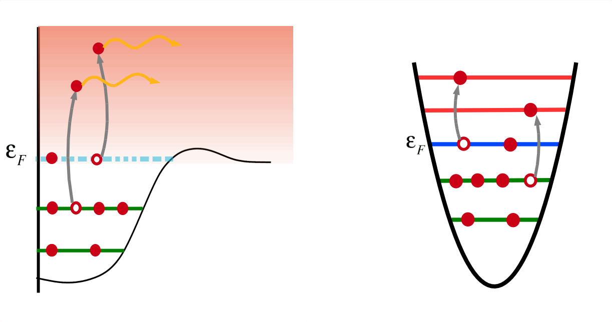
# Where we stand from an *ab initio* point of view



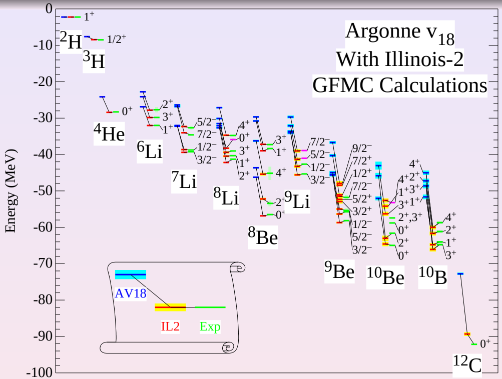
# Case 1: Halo nuclei, light nuclei and nuclear stability

**Open Quantum System.**
Coupling with continuum taken into account.

**Closed Quantum System.**
No coupling with external continuum.

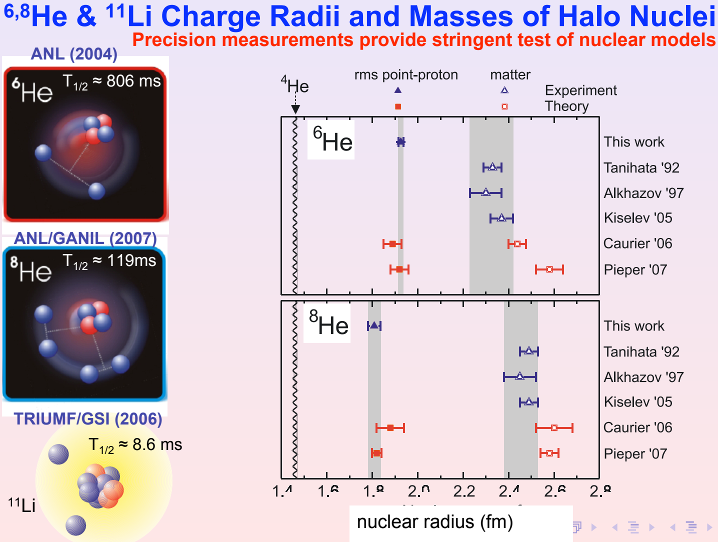


# Ab-initio approach weakly bound and unbound nuclear states



Recently also calculations of several weakly bound and light isotopes. Limit is roughly at $A \leq 12$ for Green's function Monte Carlo approaches (Pieper and Wiringa, ANL).

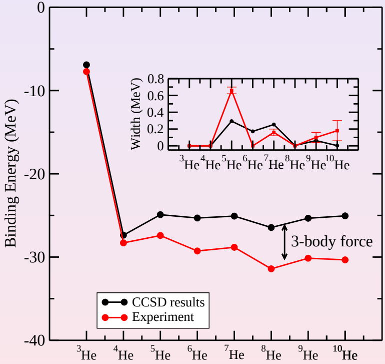
# Several experiments on light nuclei, quadrupole moments of $^{11}$Li at Isolde



## $^{6,8}$He & $^{11}$Li Charge Radii and Masses of Halo Nuclei

Precision measurements provide stringent test of nuclear models

# Coupled-cluster results for the helium chain



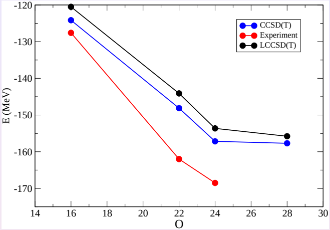
- First *ab-initio* calculation of decay widths !
- Coupled-cluster unique method for dripline nuclei.
- $\sim$ 1000 active orbitals
- Underbinding hints at missing three-body interactions?

# Oxygen Isotopes

## Several experiments worldwide

- The oxygen isotopes are the heaviest isotopes for which the drip line is well established.
- Two out of four stable even-even isotopes exhibit a doubly magic nature, namely $^{22}$O ($Z = 8$, $N = 14$) and $^{24}$O ($Z = 8$, $N = 16$).
- The structure of these two doubly magic nuclei is assumed to be governed by the evolution of the $1s_{1/2}$ and $0d_{5/2}$ one-quasiparticle states.
- The isotopes $^{25}$O $^{26}$O, $^{27}$O and $^{28}$O are outside the drip line, since the $0d_{3/2}$ orbit is not bound.
- With HIE-Isolde possible to study several O isotopes as well as selected C and N isotopes

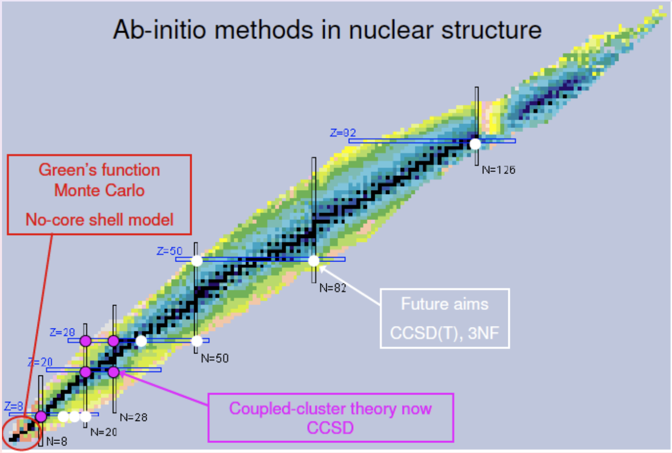
# Is $^{28}$O stable ?



- $\Lambda$CCSD(T) results for $^{28}$O indicates that it is stable towards $4n$ emission by $\sim$ 2MeV
- Results not converged with respect to model space (N=14)
- What is the binding energy of $^{26}$O ? Is this correct?

| | CCSD | | ΛCCSD(T) | |
|---|---|---|---|---|
| Nucleus | $E/A$ | $\Delta E/A$ | $E/A$ | $\Delta E/A$ |
| $^{16}$O | -6.72 | 1.25 | -7.53 | 0.44 |
| $^{22}$O | -5.72 | 1.64 | -6.59 | 0.77 |
| $^{24}$O | -5.58 | 1.42 | -6.42 | 0.58 |
| $^{28}$O | -4.86 | ? | -5.57 | ? |

# Case 2: Ab-initio approaches to light and medium mass nuclei



Ab-initio methods in nuclear structure

Green's function
Monte Carlo

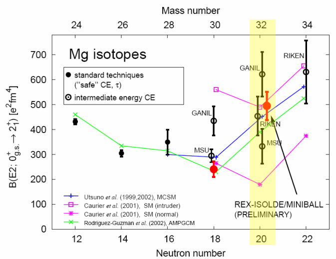
No-core shell model

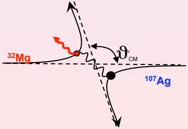
Future aims
CCSD(T), 3NF

Coupled-cluster theory now
CCSD

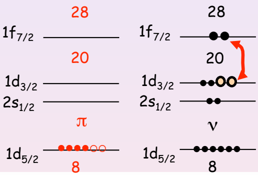
# Case 2: Island of inversion, several pioneering experiments at Isolde

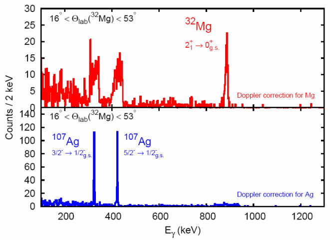
## Coulomb excitation of $^{30,32}$Mg





$^{32}$Mg = 12 π + 20 ν





*Heiko Scheit, Oliver Niedermaier, PRL 94 172501 (2005) + ISOLDE Workshop 2005-2006*

# Island of inversion (see talks by Riisager and van Duppen)

## Many experiments at Isolde

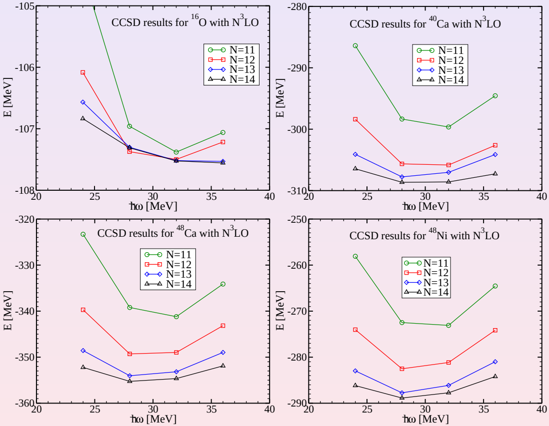
1. 2nd $0^+$ in $^{30}$Mg at 1788 keV, weak mixing, Schwerdtfeger, Thirolf et al, arXiv:0808.0264
2. $^{31}$Mg, Reiter et al (Niedermaier et al, PRL 94 (2005) 172501), coulex experiment
3. Transfer reaction d( $^{30}$Mg, $^{31}$Mg)p, Bildstein et al
4. Magnetic moments $^{30}$Mg, $^{33}$Mg, Yordanov et al, PRL 99 (2007) 212501; Kowalska et al PRC77 (2008) 034307
5. Masses, MISTRAL: Lunney et al, Eur. Phys. J. A28 (2006) 129
6. Level lifetimes: Mach et al, Eur. Phys. J. A25 (2005) 105

# Four possible Closed Shell Nuclei

## Nickel Isotopes

1. This chain of isotopes exhibits four possible closed-shell nuclei $^{48}$Ni, $^{56}$Ni, $^{68}$Ni and $^{78}$Ni.
2. Several experiments planned with different probes to test 1qp nature around $A = 56$
3. $^{48}$Ni is a presumed $2p$ emitter.
4. The challenge: can we answer which one of these is the presumably best closed-shell nucleus? How do we measure that? And which part of the nuclear forces drives it? Is it the strong spin-orbit force, the tensor force, or ..?
5. Several experiments at Isolde that map the shell-evolution for Cu, Zn, Fe and Mn isotopes.

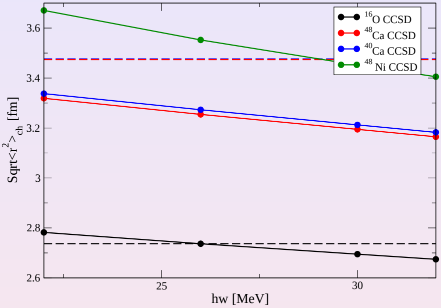
# $^{16}$O, $^{40}$Ca, $^{48}$Ca and $^{48}$Ni with “bare” chiral interactions



*Medium-Mass Nuclei from Chiral Nucleon-Nucleon Interactions*, G. Hagen et. al, Phys. Rev. Lett. 101, 092502 (2008)

# Theory up to $A = 48$

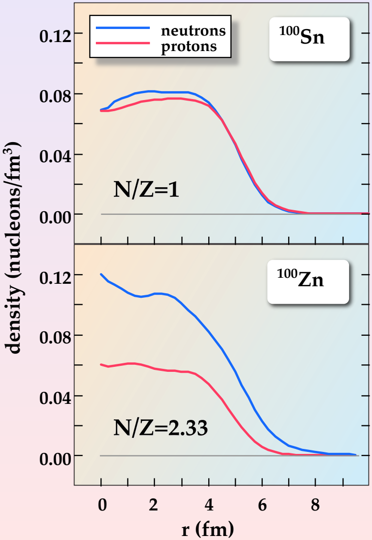
- Charge radii for various nuclei using the chiral N$^3$LO nucleon-nucleon potential.
- $\sim$ 1MeV/A missing for all nuclei: Size Extensivity!

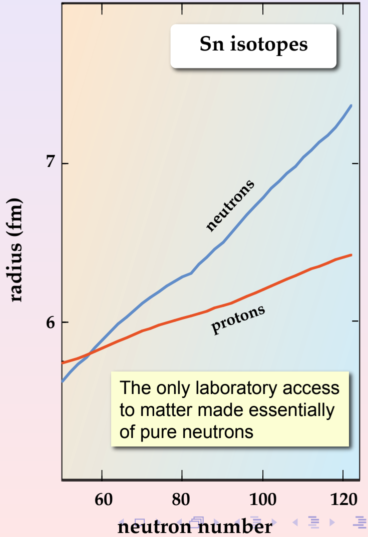


| Nucleus | $E/A$ | $V/A$ | $Q$ | $\Delta E/A$ | $< r^2 >_{ch}^{1/2}$ | $< r^2 >_{ch}^{1/2}$ $(Exp)$ |
|---|---|---|---|---|---|---|
| $^4$He | -5.99 | -22.75 | 0.90 | 1.08 | | 1.673(1) |
| $^{16}$O | -6.72 | -30.69 | 1.08 | 1.25 | 2.72(5) | 2.737(8) |
| $^{40}$Ca | -7.72 | -36.40 | 1.18 | 0.84 | 3.25(9) | 3.4764 |
| $^{48}$Ca | -7.40 | -37.97 | 1.21 | 1.27 | 3.24(9) | 3.4738 |
| $^{48}$Ni | -6.02 | -36.04 | 1.20 | 1.21 | 3.52(15) | ? |

# Case 3: Understanding nuclei around $A = 100$

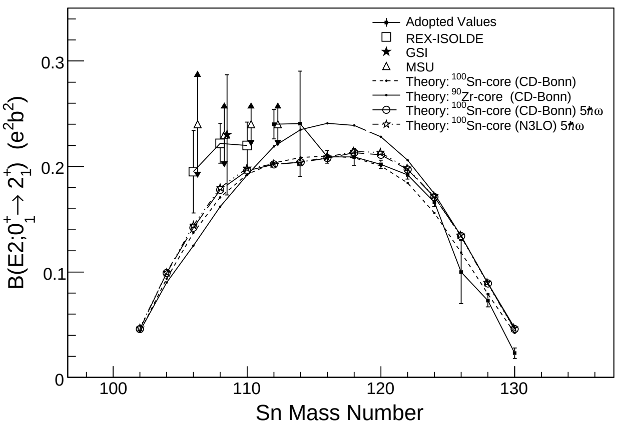
## Neutron skins



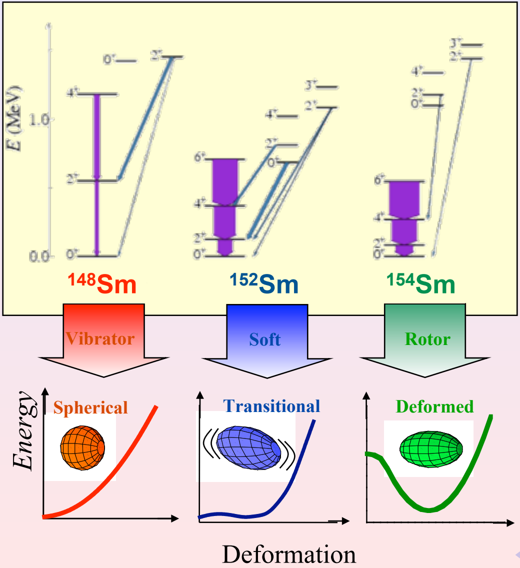


The only laboratory access to matter made essentially of pure neutrons

# Electromagnetic transitions, pioneering Coulex experiments at Isolde



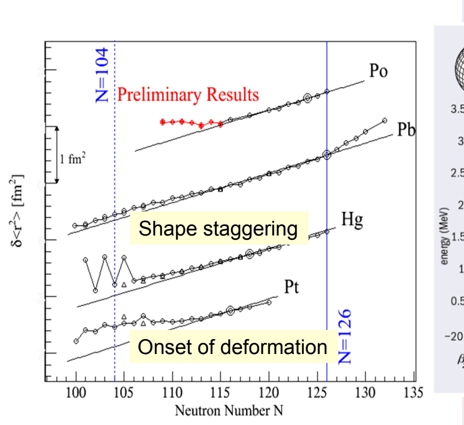
# Case 4: Shape coexistence and transitions



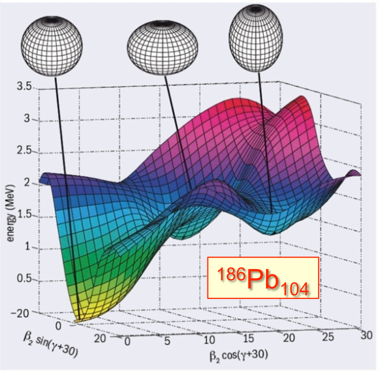
## Challenges for theory

- Possible shape transitions, huge spaces needed to describe properly.
- Theory: need to marry *ab initio* methods with density functional theories in order to describe such systems
- Need a large wealth of experimental data to constrain theory

# Case 4: Shape coexistence in lead isotopes, Isolde experiments (see talk by van Duppen)



H. De Witte et al. PRL 98 (2007) 112501

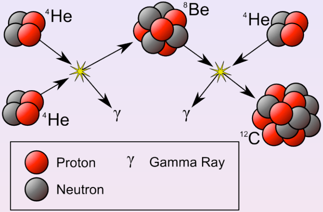


A.N. Andreyev et al., Nature 405, 430 (2000)

# Case 5: Nuclear astrophysics

## 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
- 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]



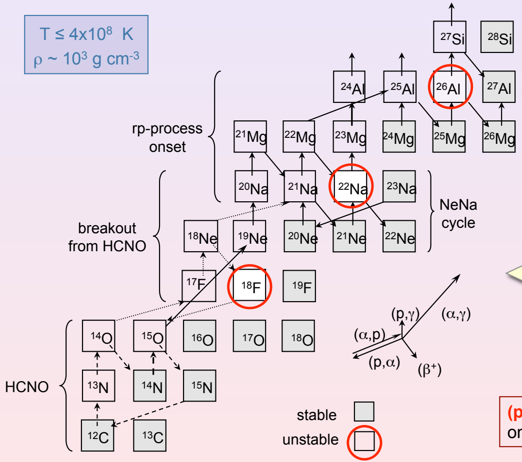
## $^{12}$C and nucleonsynthesis

- $^{12}$C resonances studied at Isolde, Nature (2005)
- crucial for understanding the CNO cycle.

# From $^{12}$C to $A = 40$

## Novae: nucleosynthesis up to A ~ 40 mass region

$T \leq 4\times10^{8}$ K
$\rho \sim 10^{3}$ g cm$^{-3}$



rp-process onset

breakout from HCNO

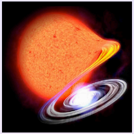
NeNa cycle

HCNO

stable ☐

unstable ○

observable long-lived nuclei



nova
(artist's impression)

reaction network for explosive hydrogen burning

**(p,γ)** and **(α,p)** reactions on proton-rich nuclei

# Summary: much Work in Progress

- Strong ties theory and experiment needed
- Three-body forces included routinely in ab initio methods
- Can now extract effective interactions for the nuclear shell-model, with and without three-body forces.
- Inclusion of continuum effects, can study weakly bound systems.
- First studies combining reaction and structure theory by no-core-shell-model collaboration
- Ground state properties of closed-shell nuclei, from $^4$He to $^{208}$Pb: Now $^{56}$Ni and possibly $^{100}$Sn. Nuclear matter calculations within reach.
- Can we understand how shells evolve? Is it due to three-body effects or continuum effects, or something else?

# Future theory directions

- Effective field theories are the natural bridge between LQCD and nuclear structure/reactions.
- For heavier nuclei large ongoing collaborations on density functional theories. Can we link these with present ab initio approaches? Crucial for studies of shape coexistence
- Mandatory to marry reaction theories with structure calculations. Very interesting work by the no-core shell-model and Green's function Monte Carlo collaborations
- Develop new algorithms for the nuclear many-body problem, exploiting development in parallel computing facilities. Petascale:now, Exascale: $t < 10$ yr. Need to effectively utilize both core speed and memory to attack nuclear problems.
- Measure of success: predictive nuclear theory in medium-mass nuclei (to mass 208).
- Produce better effective interactions for the shell-model.
- Develop common computing tools which can aid in training of students and in performing data analysis.

# ORNL-OSLO Many-Body project

## ORNL

David Dean, Gaute Hagen, Thomas Papenbrock

## Oslo

Elise Bergli, Torgeir Engeland, Morten Hjorth-Jensen, Gustav Jansen, Maxim Kartamychev, Simen Kvaal and Eivind Osnes

## And this meeting

Many thanks to Yorick Blumefeld, Peter Butler, Mark Huyse, Karsten Riisager and Piet van Duppen

# Coupled Cluster Theory

## Exponential Ansatz for Ψ

$$|\Psi\rangle = e^{\hat{T}}|\Phi_0\rangle, \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$

$$\hat{T}_1 = \sum_{i,a} t_i^a \hat{a}_a^\dagger \hat{a}_i, \quad \hat{T}_2 = \frac{1}{2} \sum_{i<j,a<b} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i.$$

## Coupled Cluster Equations

$$\Delta E = \langle \Phi_0 | \left( H_N exp(T) \right)_C | \Phi_0 \rangle$$

$$0 = \langle \Phi_p | \left( H_N exp(T) \right)_C | \Phi_0 \rangle$$

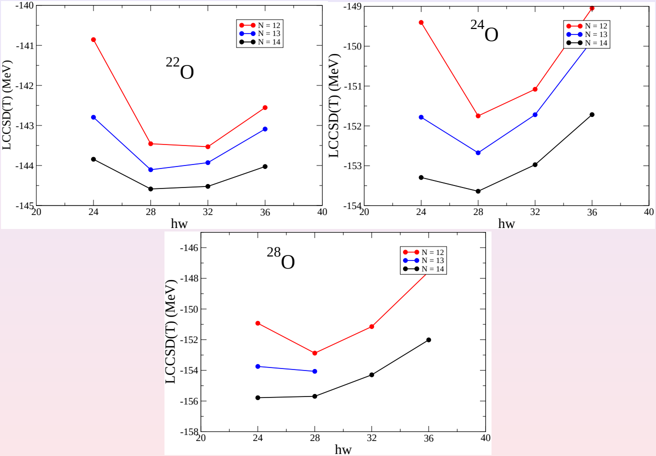
$$\bar{H} = \left( H_N exp(T) \right)_C$$

1. Coupled Cluster Theory is fully microscopic .
2. Coupled Cluster is size extensive. No unlinked diagrams enters, and error scales linearly with number of particles.
3. Low computational cost (CCSD scales as $n_o^2 n_u^4$).
4. Capable of systematic improvements.
5. Amenable to parallel computing.

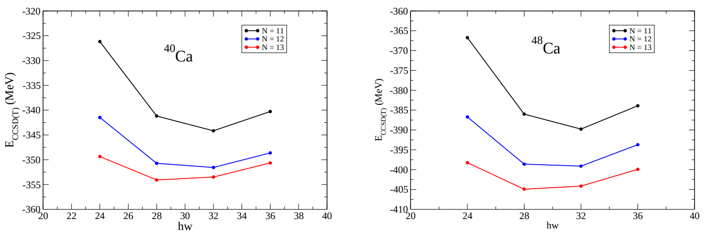
# Spherical Coupled-Cluster Approach

1. Possible for nuclei with closed sub-shell (or cs ±1 and cs ±2)
2. Relatively simple since similarity transformed Hamiltonian is two-body (CCSD) or three-body (CCSDT) at most
3. Enourmous computational reduction: $n_o + n_u \rightarrow (n_o + n_u)^{2/3}$ (naive estimate)
   CCSD(T) for $^{40}$Ca and $^{48}$Ca on a single CPU (now)
   CCSDT for $^{48}$Ca on many CPUs (soon)
   CCSD(T) for $^{100}$Sn and $^{132}$Sn with "bare" chiral interactions on many CPUs (summer/fall 2009).

# $^{22}$O, $^{24}$O, and $^{28}$O with chiral interactions



# Triples correction to ground state energies



- $\sim$ 500keV/A missing for all nuclei
- Chiral interactions leaves almost no room for three-body forces in medium size nuclei.

| | CCSD | | ΛCCSD(T) | |
|---|---|---|---|---|
| Nucleus | $E/A$ | $\Delta E/A$ | $E/A$ | $\Delta E/A$ |
| $^{16}$O | -6.72 | 1.25 | -7.53 | 0.44 |
| $^{40}$Ca | -7.72 | 0.84 | -8.62 | -0.08 |
| $^{48}$Ca | -7.40 | 1.27 | -8.22 | 0.45 |