The nuclear many-body problem

David J. Dean
Oak Ridge National Laboratory

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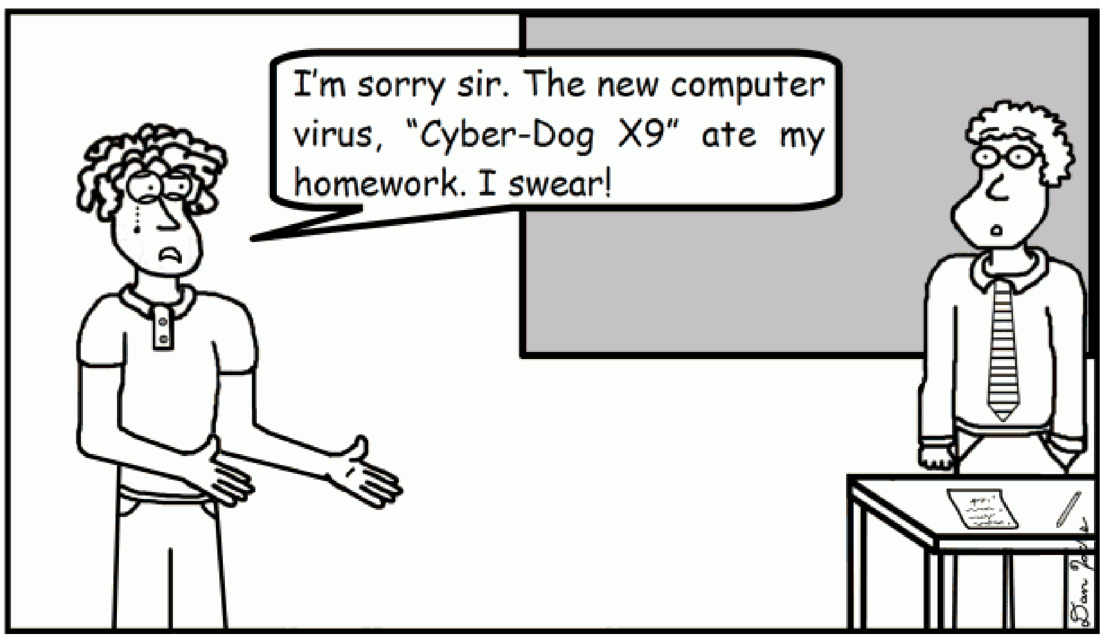
"Fair and Balanced"

I'll try to teach a liberal dose of conservative art.

Caveat: 4 hours == high selectivity

Yes, we do value the computational sciences.

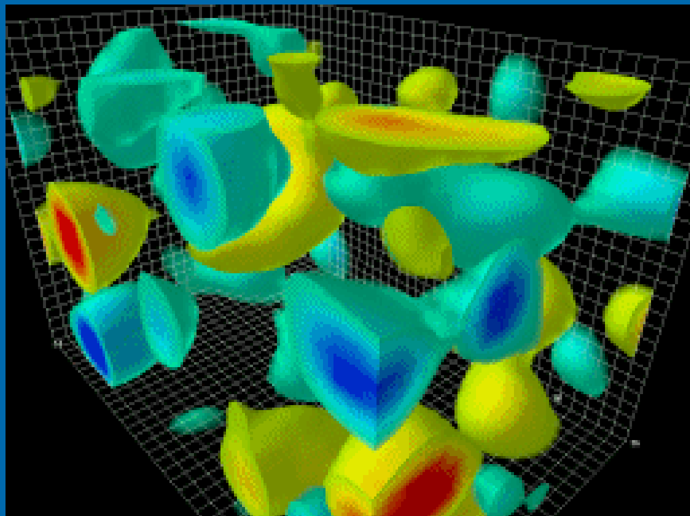


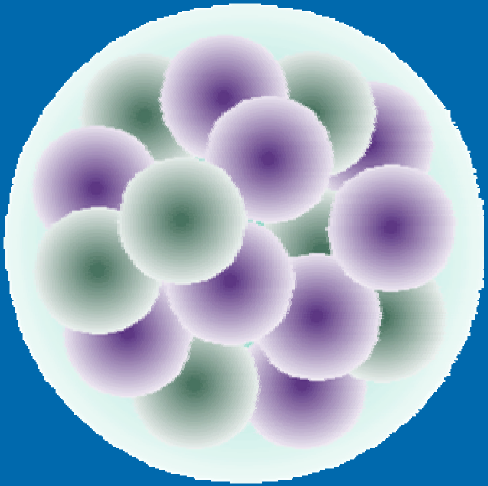
"Somethings never change!"

We will cover some generalities today (lecture 1)

- **General questions in nuclear physics**
- **Shell structure in nuclei**
- **Implications for nucleosynthesis**
- **Nuclear impacts on type-II supernova**
- **neutrinoless $\beta\beta$-decay**

Nuclear Physics Today



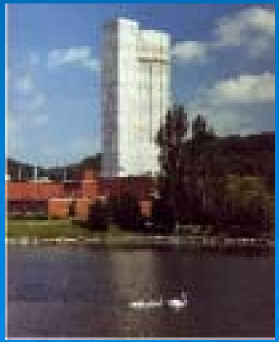


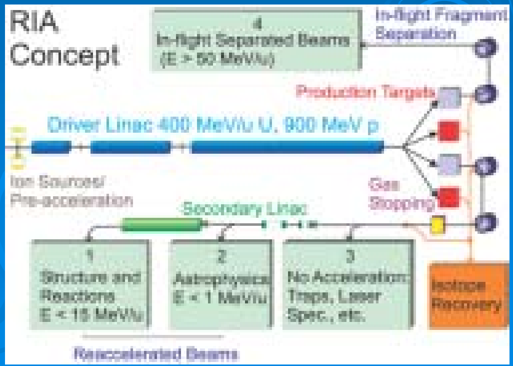
- What is the nature of the quark-gluon matter?
- Where is the glue that binds quarks into strongly interacting particles, and what are its properties?
- What is the internal landscape of the proton?
- What does QCD predict for the properties of nuclear matter?

- What binds protons and neutrons into stable nuclei and rare isotopes?
- What is the origin of simple patterns in complex nuclei?
- When and how did the elements from iron to uranium originate?
- What causes stars to explode?

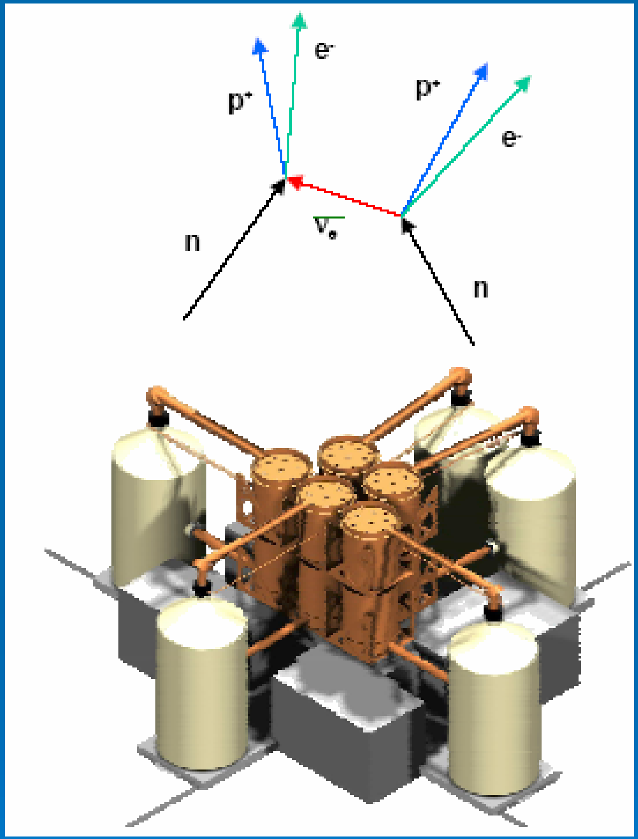
Brookhaven National Lab. **RHIC**

Thomas Jefferson National Accelerator Facility: **CEBAF**



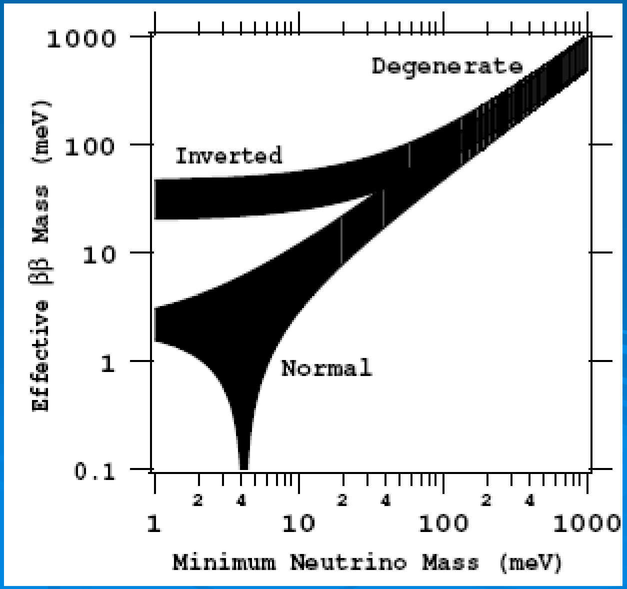


Nuclear Physics Today



- What are the masses of neutrinos and how have they shaped the evolution of the universe?
- Why is there more matter than antimatter?
- What are the unseen forces that disappeared from view as the universe cooled?

For many of these experiments nuclei are used as laboratories to probe 'beyond standard model' science.



Is the neutrino it's own anti-particle? Is it a Majorana or Dirac particle?

"Given a lump of nuclear material, what are its properties, how did it get here, and how does it react?"

How are we going to describe nuclei that we cannot measure?

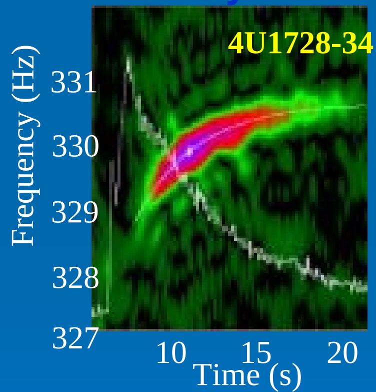
→Robust and predictive nuclear theory

→Need for nuclear data to constrain theory

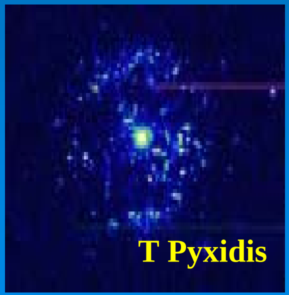
→We are after the Hamiltonian

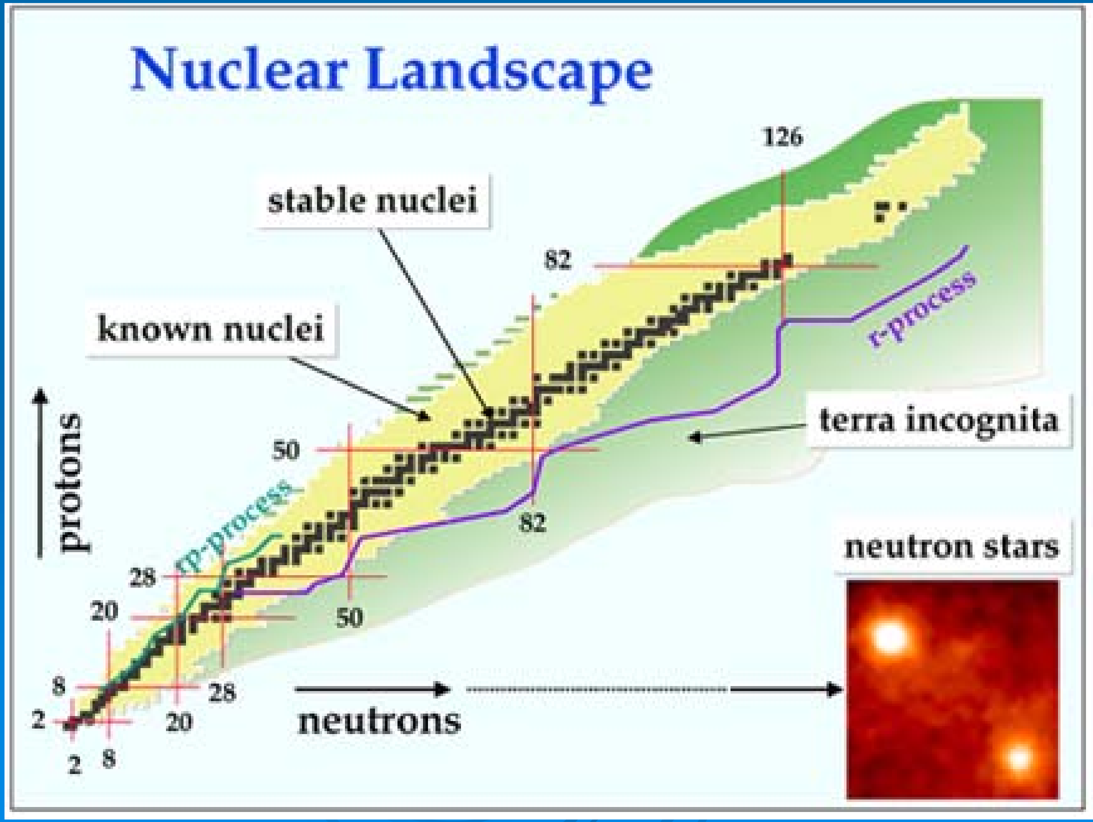
- →bare intra-nucleon Hamiltonian
- →energy density functional

X-ray burst

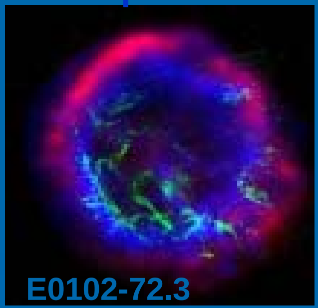


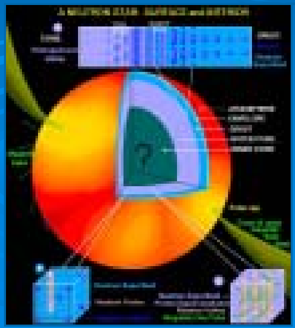
Nova





Supernova





Uncorrelated basis states: Harmonic Oscillators

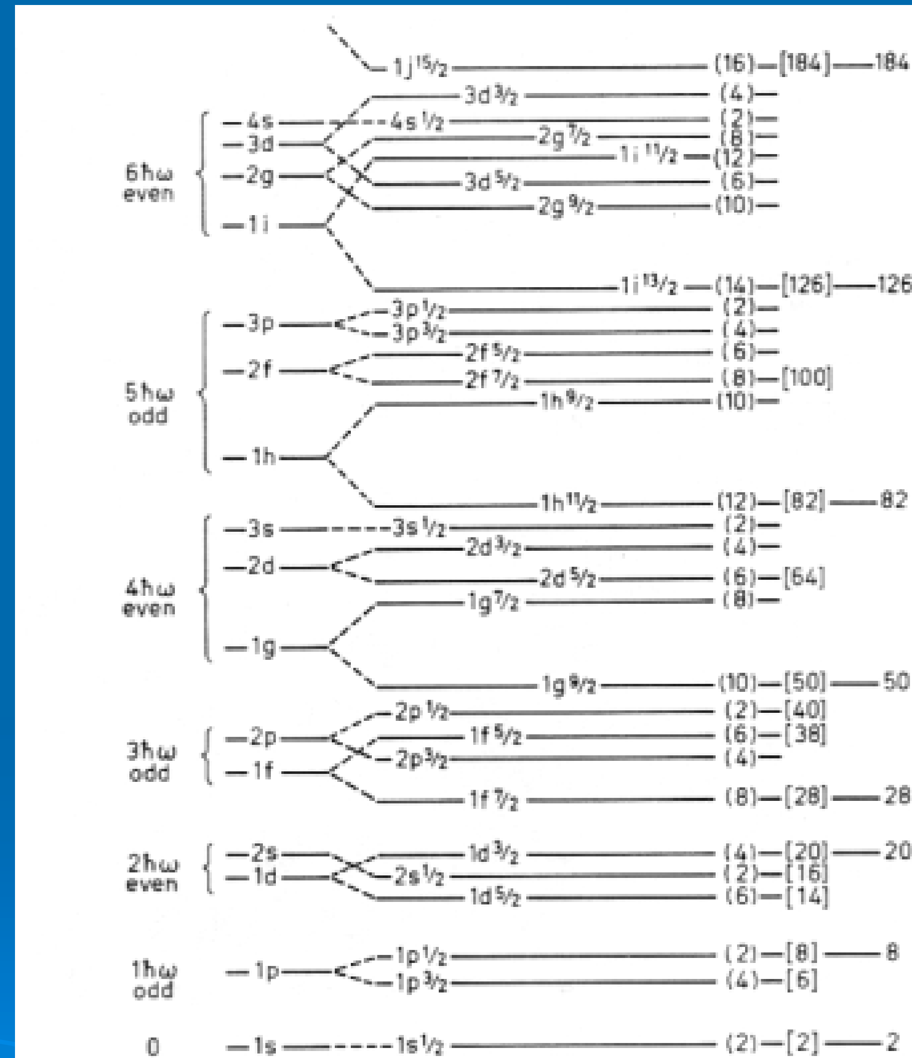
$$H_0 = \sum_{i=1}^{A} \left(\frac{\hbar^2}{2M} \nabla^2 + \frac{m}{2} \omega^2 r^2 \right)$$

$$E = \hbar\omega(2n + l - 1/2)$$
$$\varphi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\vartheta, \varphi)$$
$$R_{nl}(r) \sim r^l e^{-r^2} \times \left[\text{hypergeometric function in } r^2\right]$$

Couple to spin-1/2 (LS)

$$\varphi_{nljj_z}(\vec{\mathrm{r}}) = R_{nl}(r) \left[Y_l(\hat{\mathrm{r}}) \otimes \chi^S_{\frac{1}{2}} \right]^{jj_z}$$
$$\left[Y_l(\hat{\mathrm{r}}) \otimes \chi^S_{\frac{1}{2}} \right]^{jj_z} = \sum_{ms_z} \left(lm \tfrac{1}{2} s_z \mid jj_z \right) Y_{lm}(\hat{\mathrm{r}}) \chi^S_{\frac{1}{2} s_z}$$

$$\left| \phi_\alpha \right\rangle = \left| nljmt_z \right\rangle \qquad j = l + 1/2$$



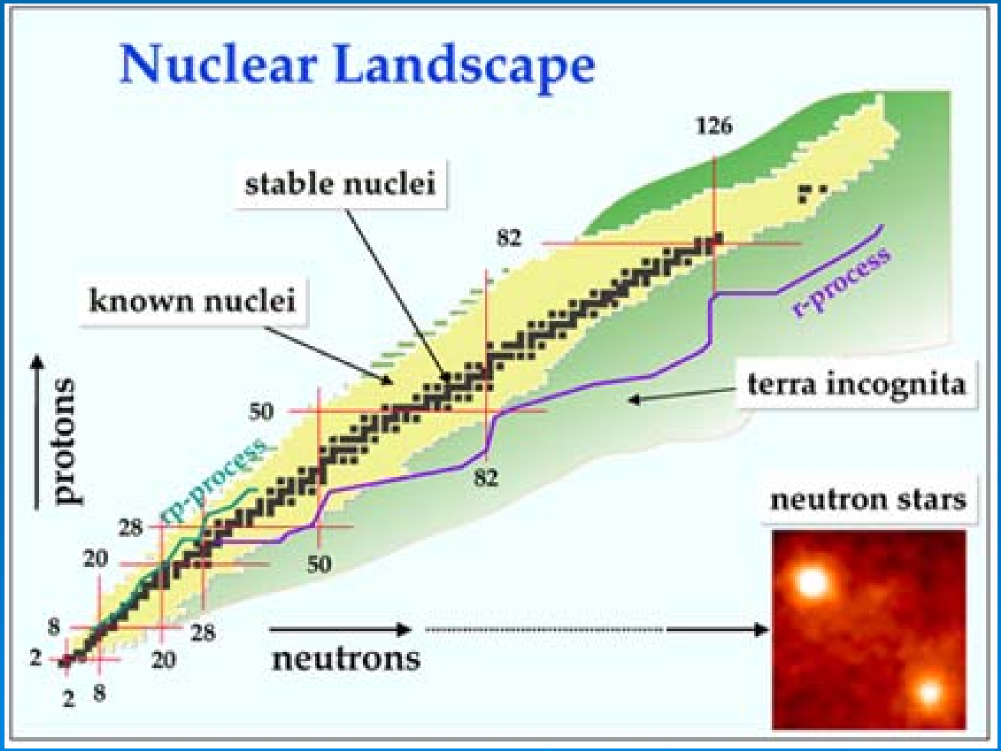
$$H_{SM} = \sum_{i=1}^{A} \left(\frac{\hbar^2}{2M} \nabla^2 + \frac{m}{2} \omega^2 r^2 + \eta_l \vec{l}^{\,2} + \xi_{ls} \vec{l} \bullet \vec{s} \right)$$

Shell structure in nuclei: then and now

$$H_{SM} = \sum_{i=1}^{A}\left(\frac{\hbar^2}{2M}\nabla^2 + \frac{m}{2}\omega^2 r^2 + \eta_l \vec{l}^{\,2} + \xi_{ls}\vec{l}\bullet\vec{s}\right)$$

The Nobel Prize in Physics 1963

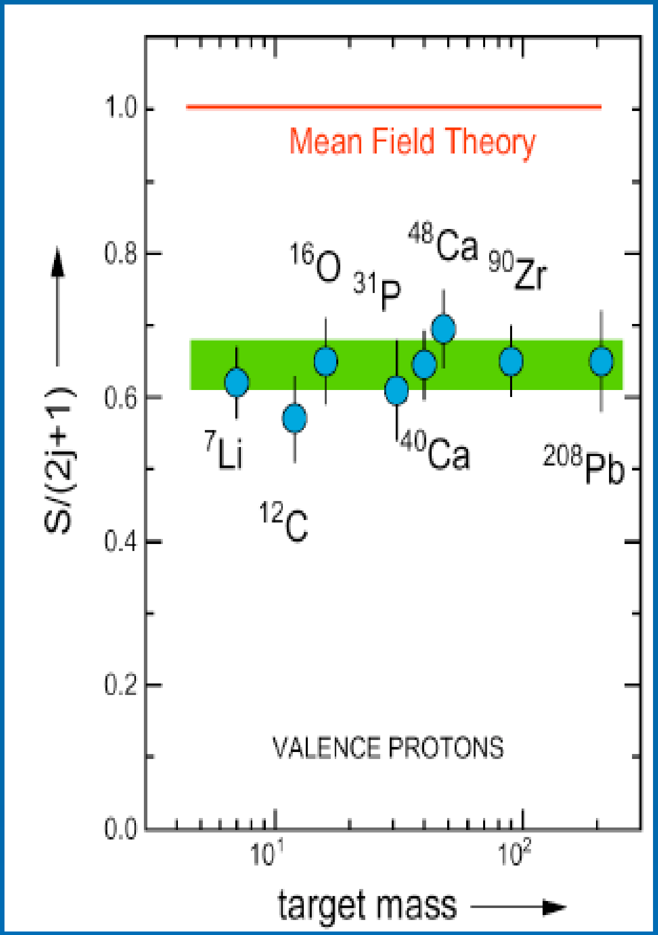
Maria Goeppert-Mayer J. Hans D. Jensen



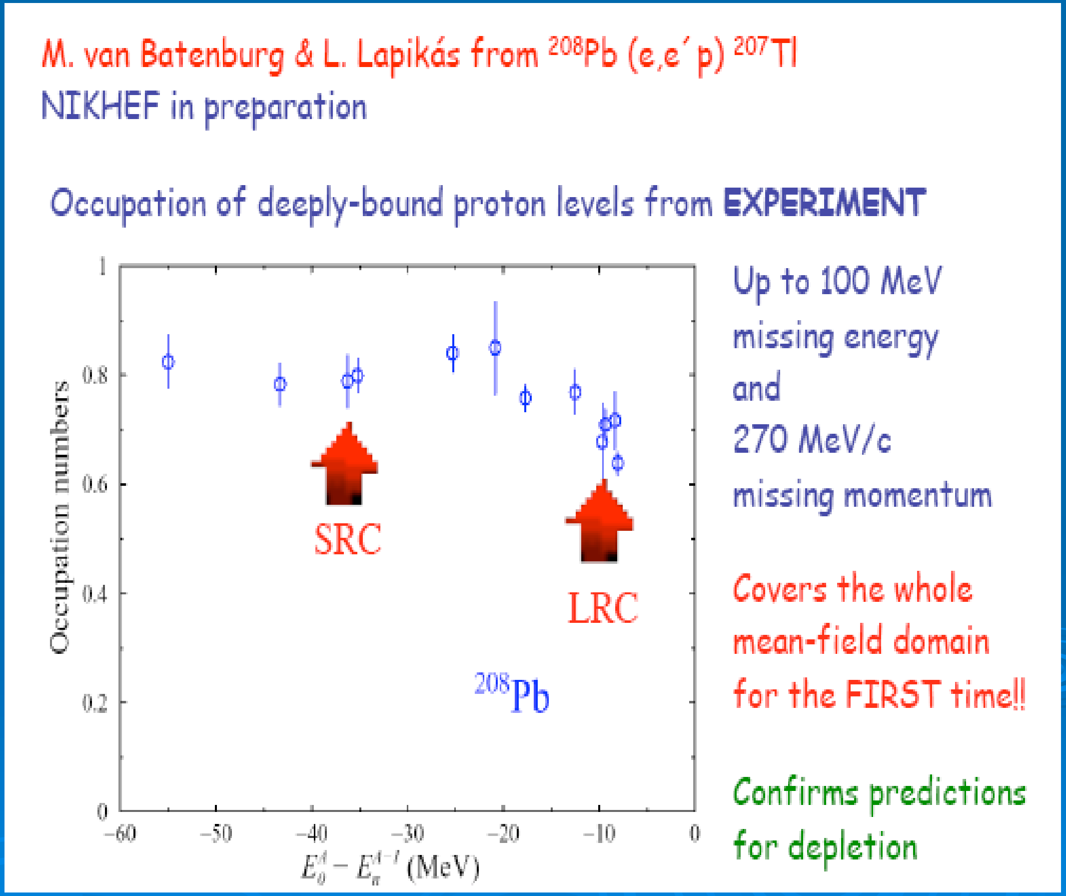
Red lines denote 'magic' numbers.

Is this the end of the story?

NO – definitely not.

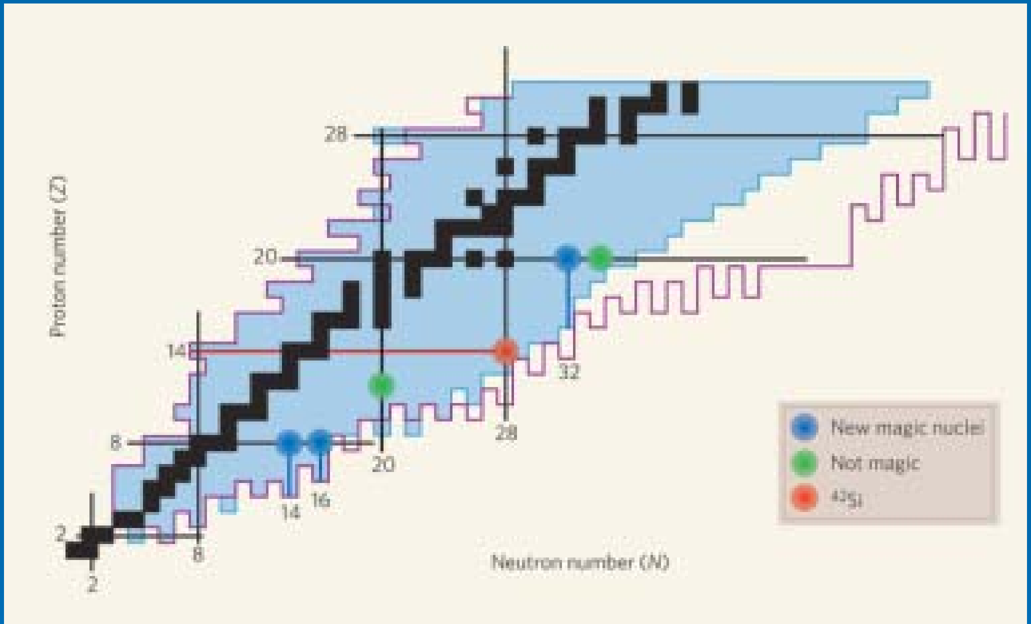


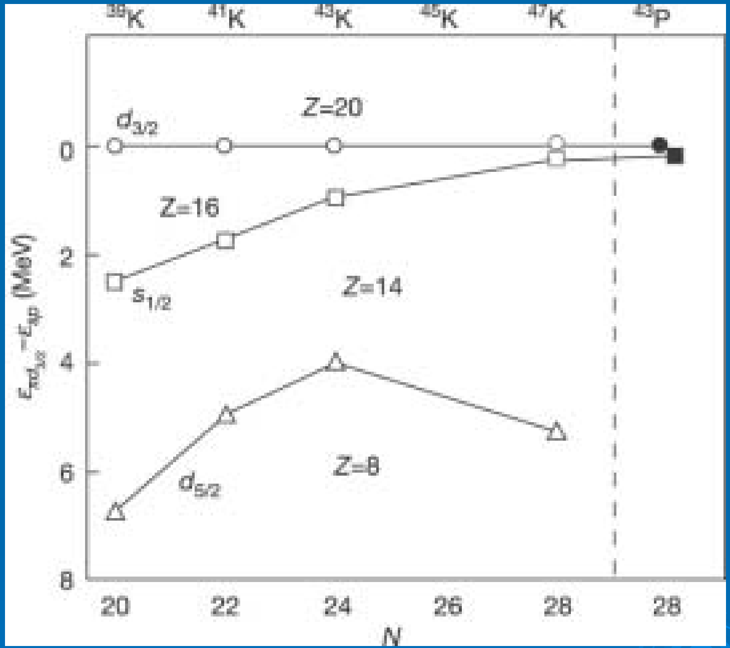
While we will discuss 'closed shells' one should note that shells are not really all that closed.



Does shell structure change in unstable nuclei?

Fridmann et al., Nature 435, 922 (2005)
(comment) Jansens, Nature 435, 207 (2005)



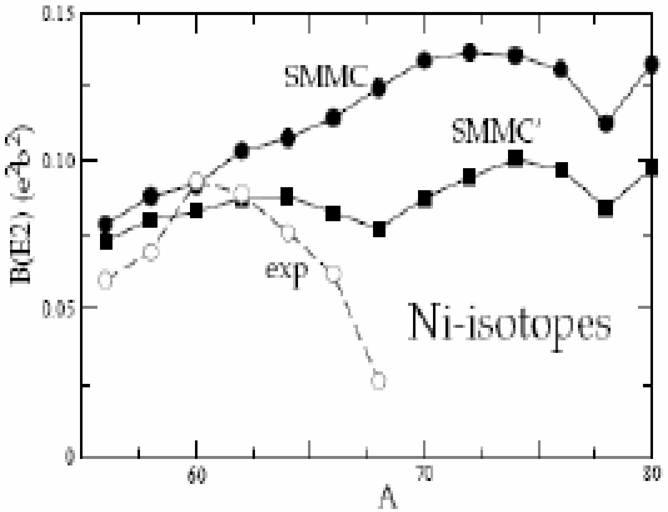


Answer: Yes indeed. Magic numbers fluctuate when one moves away from stability!!!

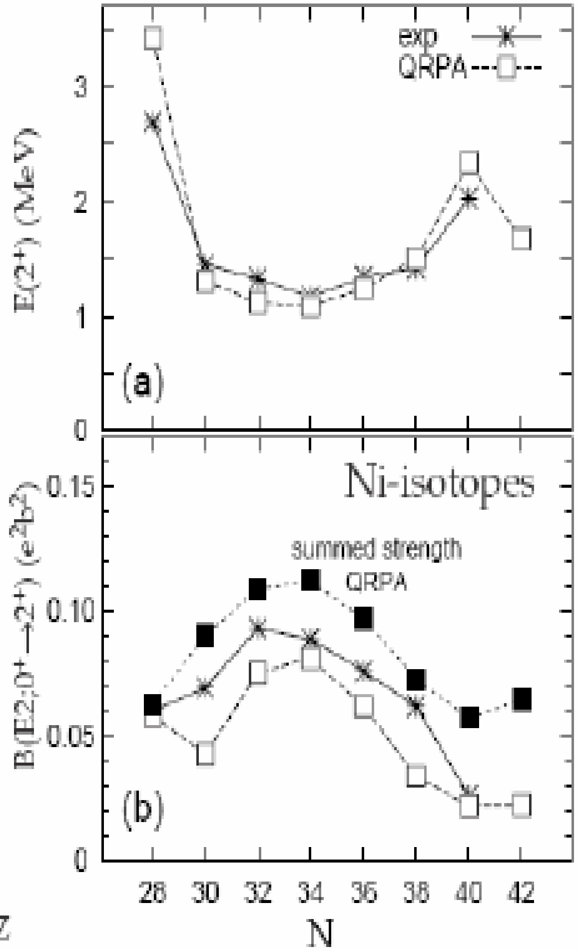
N=40 – How magic is the magic ^{68}Ni nucleus?

- low-lying 0^+_2 level
- higher energy of the 2^+_1
- small value of $B(E2, 0^+_1 \rightarrow 2^+_1)$

interpreted as evidence for magicity!



Shell-model Monte-Carlo total summed B(E2) strength to the 2^+ excited states.



LANGANKE, TERASAKI, NOWACKI, DEAN, AND NAZAREWICZ
PHYSICAL REVIEW C 67, 044314

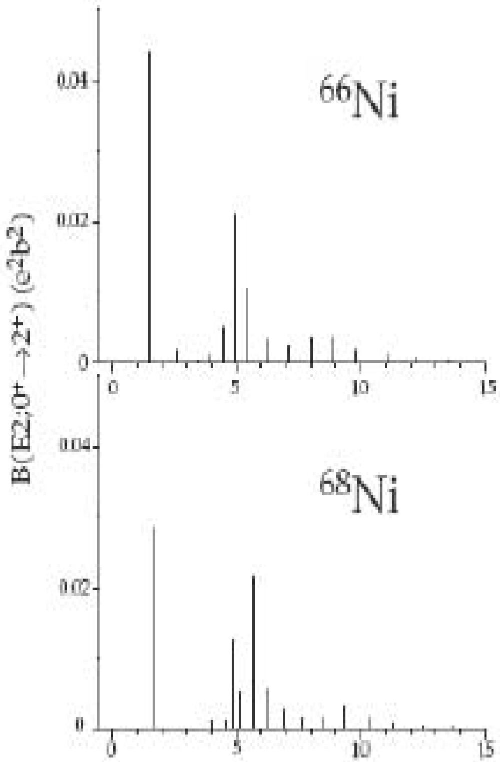
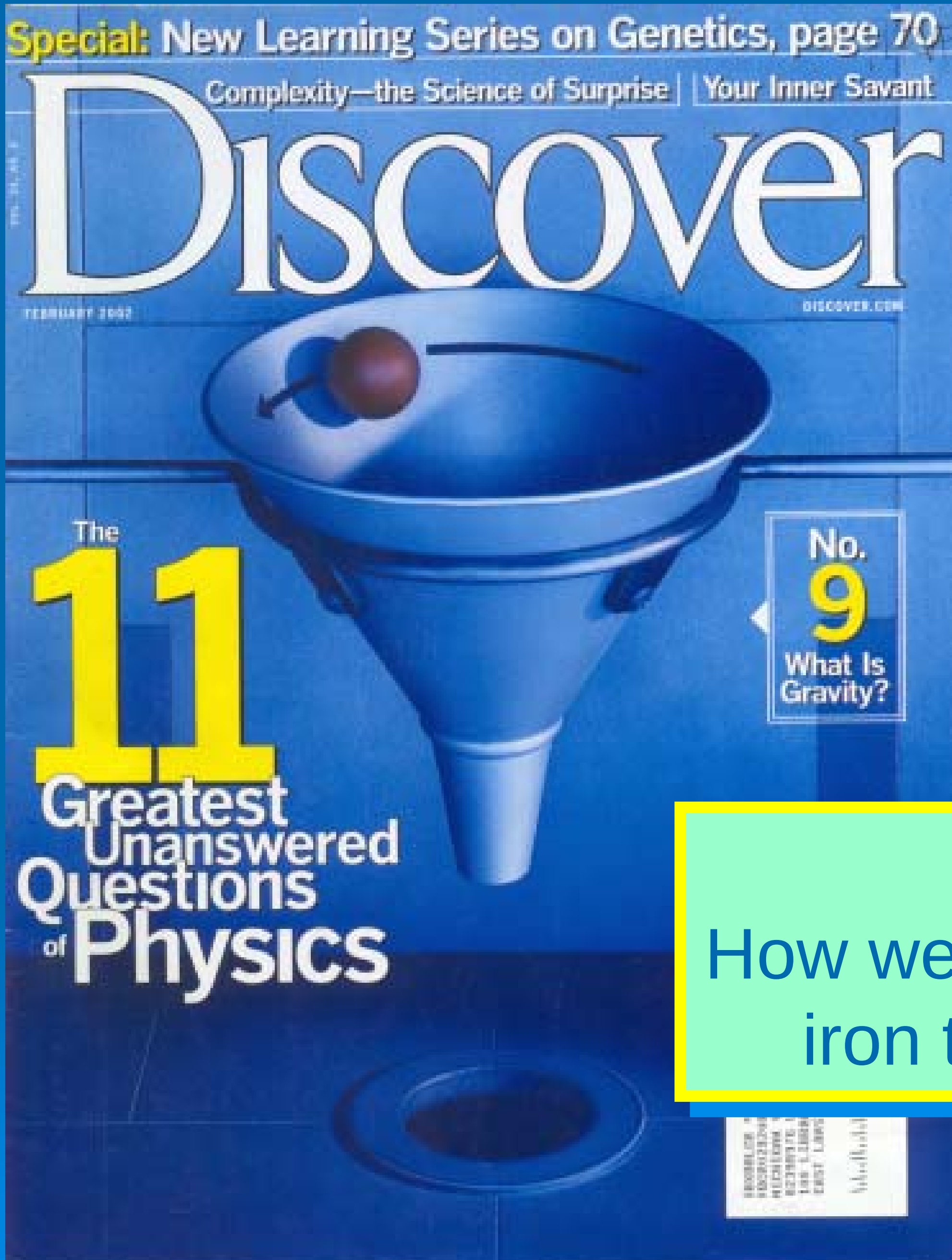


FIG. 4. Distribution of the $B(E2; 0^+_{g.s.} \rightarrow 2^+)$ strength in ^{66,68}Ni calculated in the diagonalization shell model.

Shell-model Monte-Carlo, QRPA and large-scale diagonalization shell-model calculations have shown that the B(E2) transition to the first 2^+ state exhaust only a fraction of the low-lying B(E2) strength.

Small B(E2) value to the first 2^+ state is not a strong evidence for the doubly magic character of ^{68}Ni.



Based on National Academy of Science Report

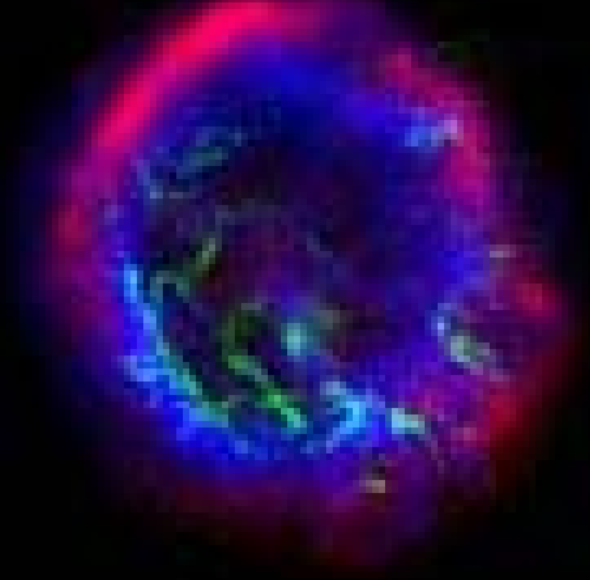
[Committee for the Physics of the Universe (CPU)]

Question 3

How were the elements from iron to uranium made ?

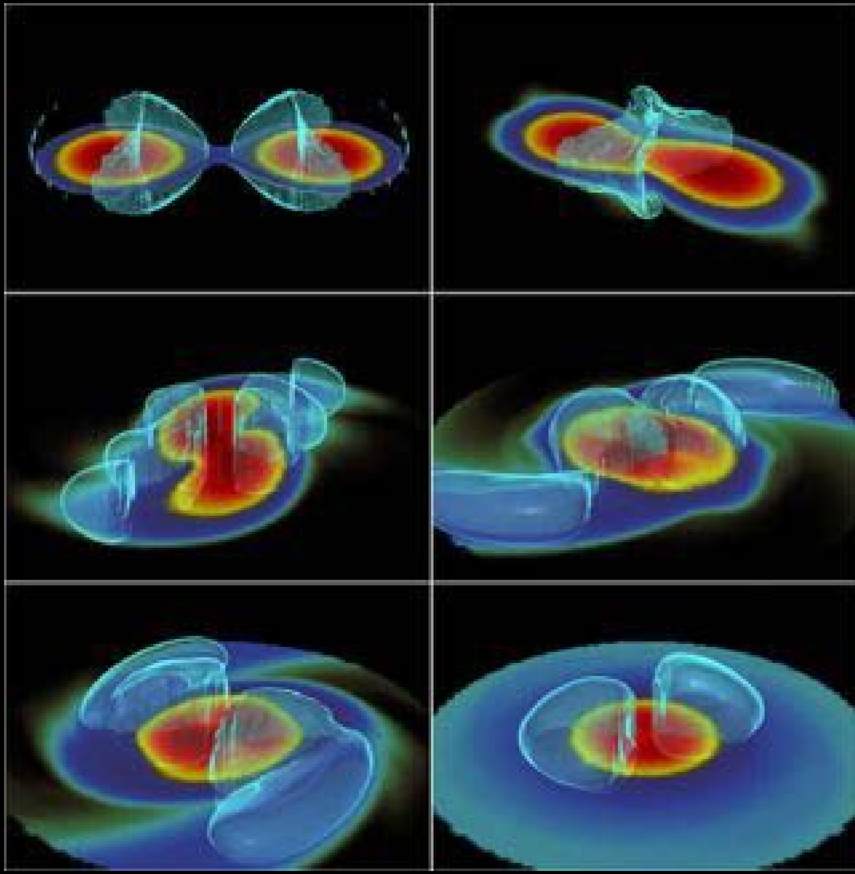
r (apid neutron capture) process

Supernovae ?



The origin of about half of elements > Fe (including Gold, Platinum, Silver, Uranium)

Neutron star mergers ?



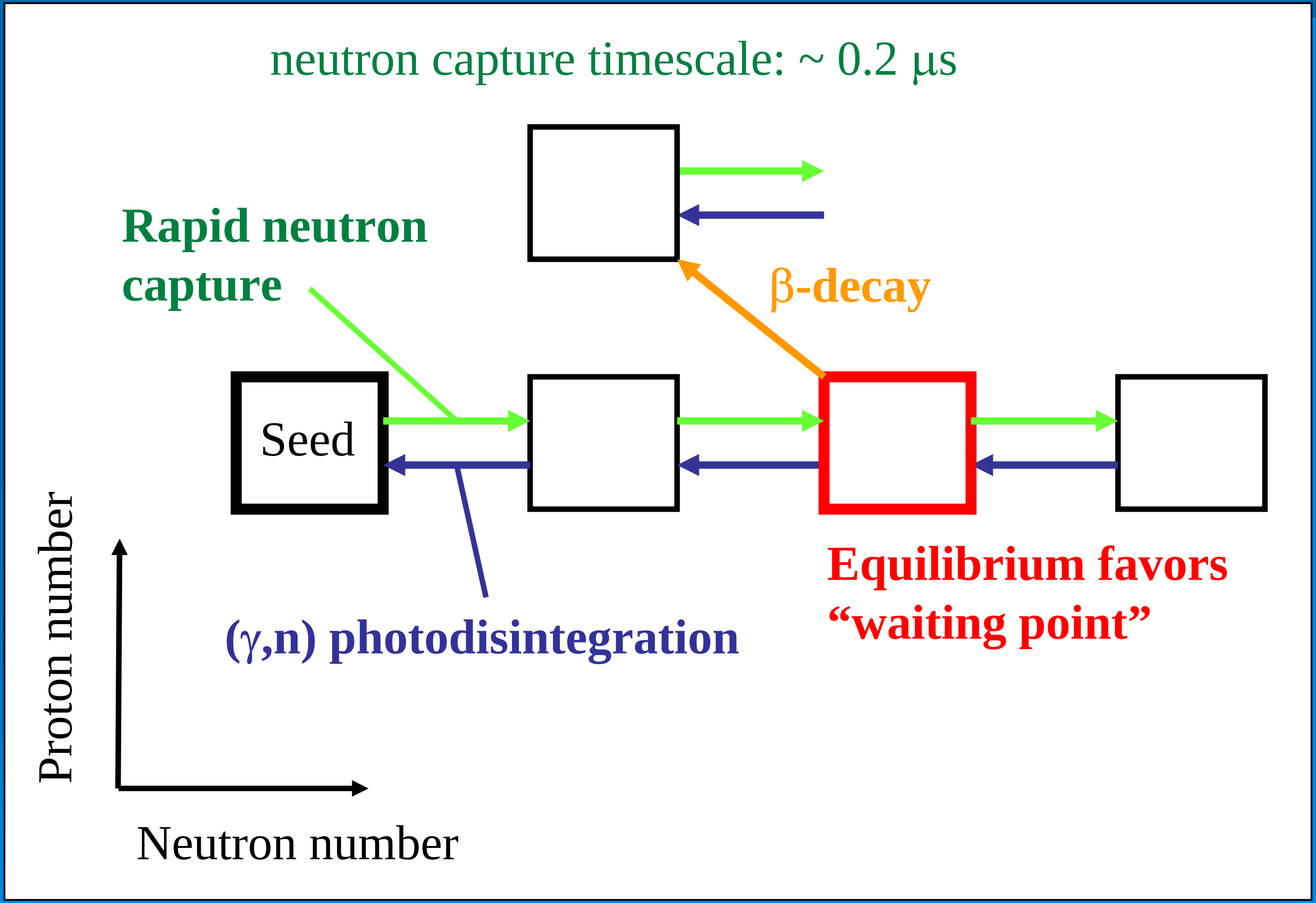
Swesty, Calder, Wang

Open questions:

- Where does the r process occur ?
- New observations of single r-process events in metal poor stars
- Can the r-process tell us about physics under extreme conditions ?

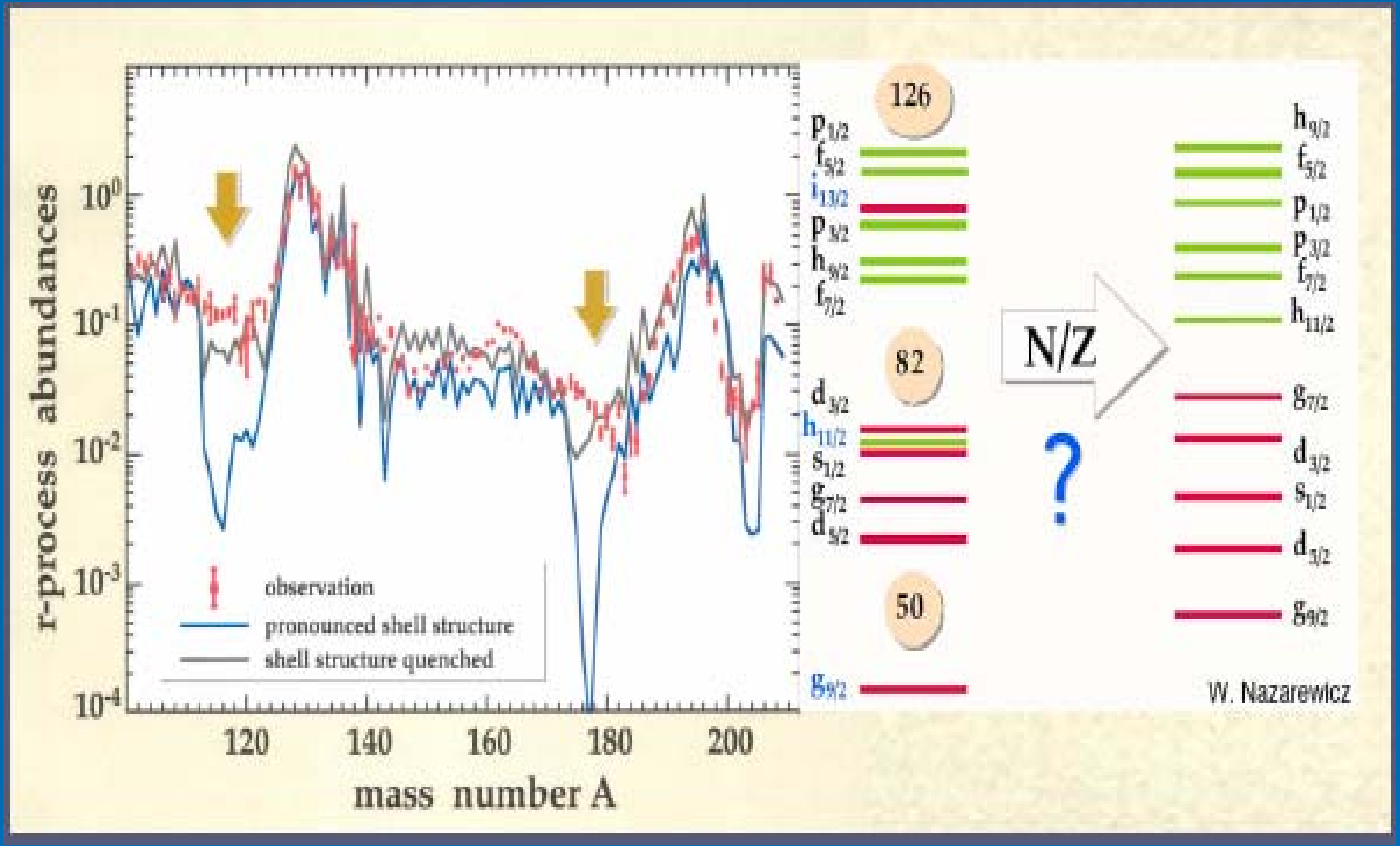
Challenge: when and how did elements from Fe to U originate?

Input: masses, density of states, single-particle energies, shapes, beta-decay values, optical potential, ….!



r-process movie

Does this potential changing of shell structure have consequences?

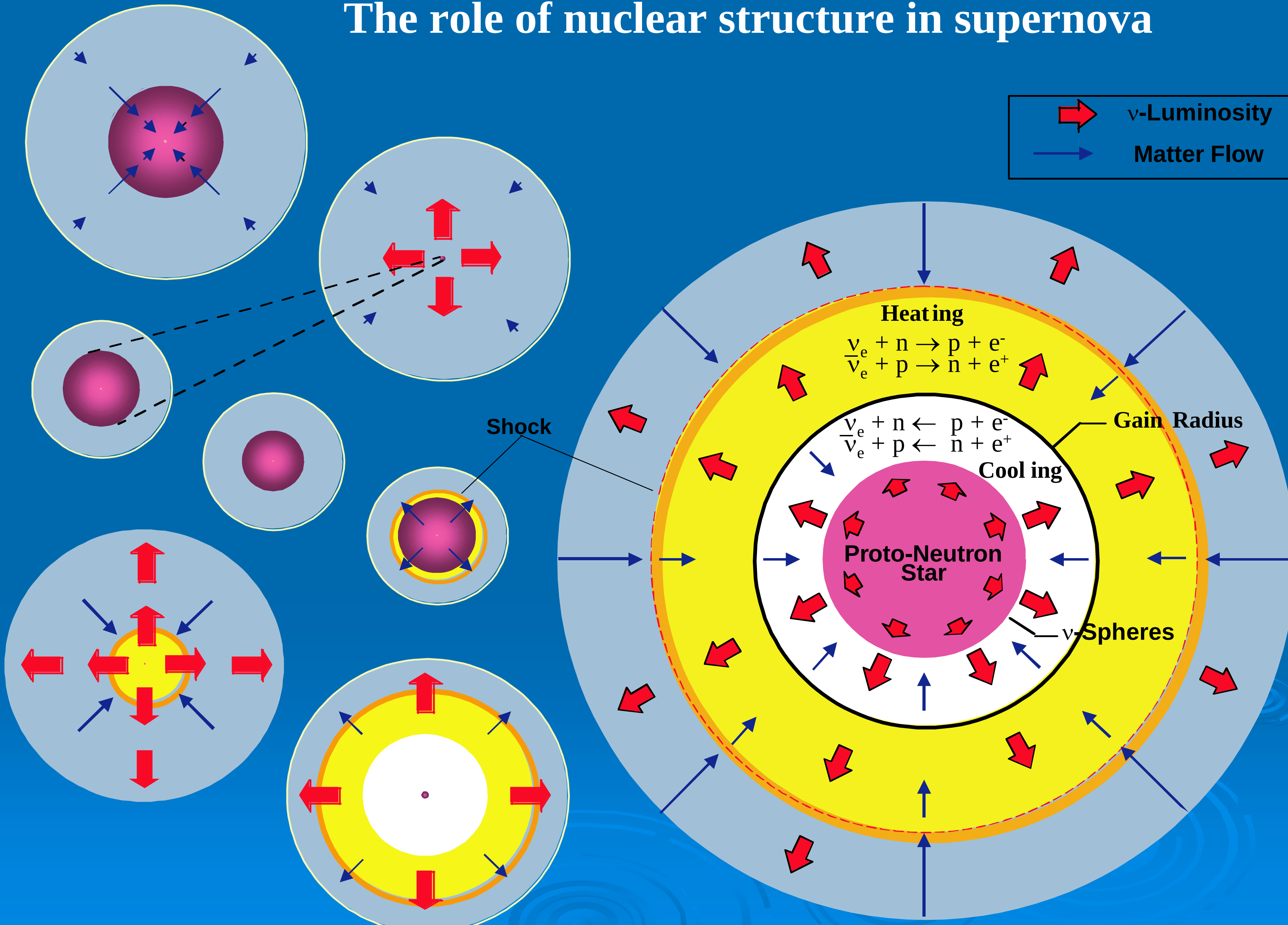


Possibly…. Such changes in abundances could also be due to

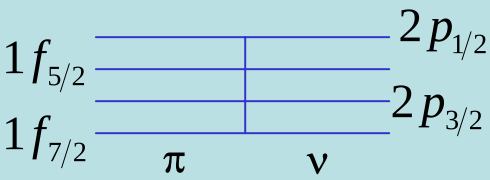
a) unaccounted neutrino nucleosynthesis

b) signature of underestimated beta-delayed neutron decay

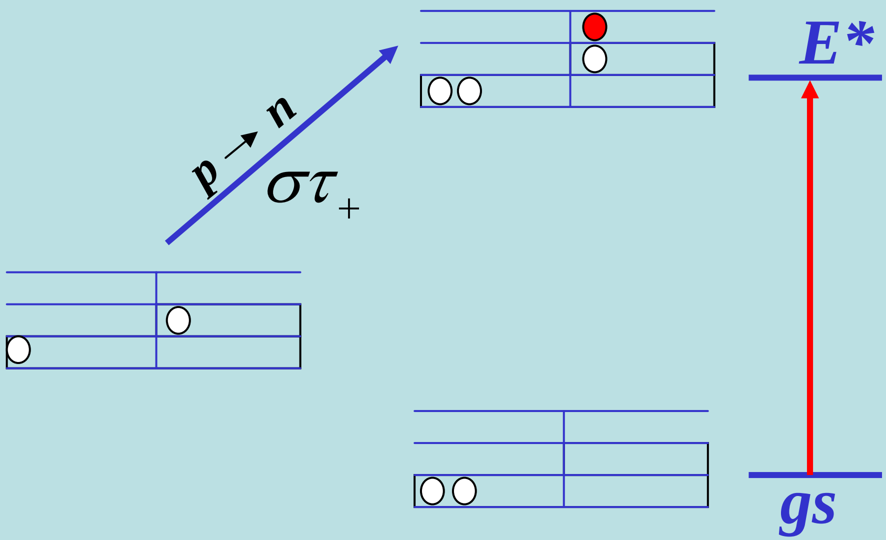
The role of nuclear structure in supernova

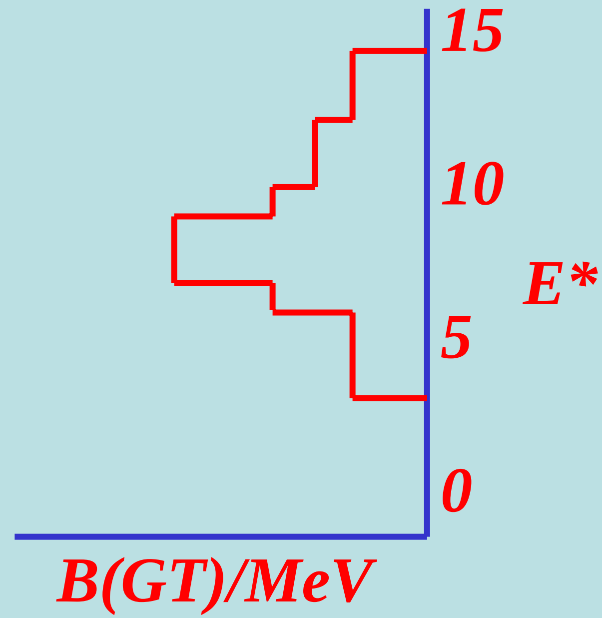


Core collapse implications of e-capture on nuclei



$$e^- + A(Z,N) \rightarrow A(Z-1,N+1) + \nu_e$$



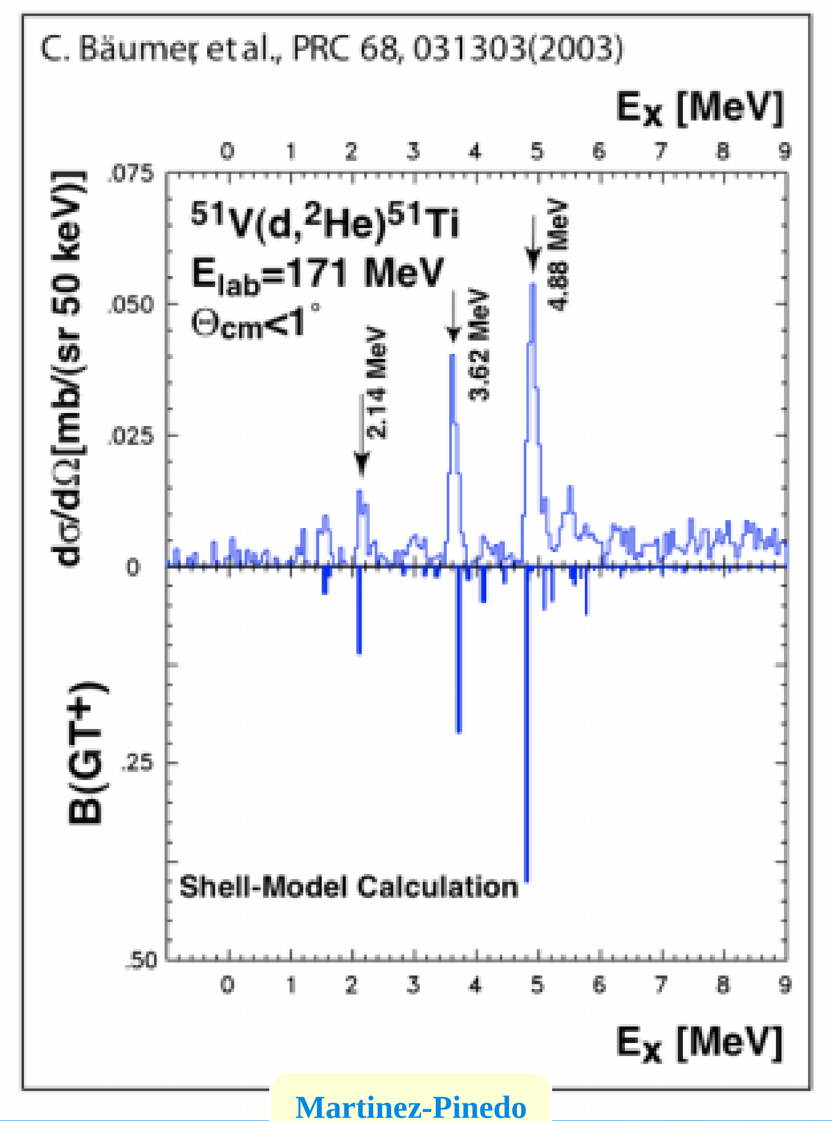


$$B(GT_+) = \sum_{i,k} \frac{n_p(i)\bar{n}_n(k)}{2j_k+1} \left| \langle i | \sigma\tau_+ | f \rangle \right|^2$$ **(FFN phenomenology)**

Koonin, Dean, Langanke, Phys. Rep. 278, 1 (1997)
Radha, Dean, Koonin, Langanke, Vogel, Phys. Rev. C56, 3079 (1997)
Langanke, Martinez-Pinedo, NPA 673, 431 (2000)

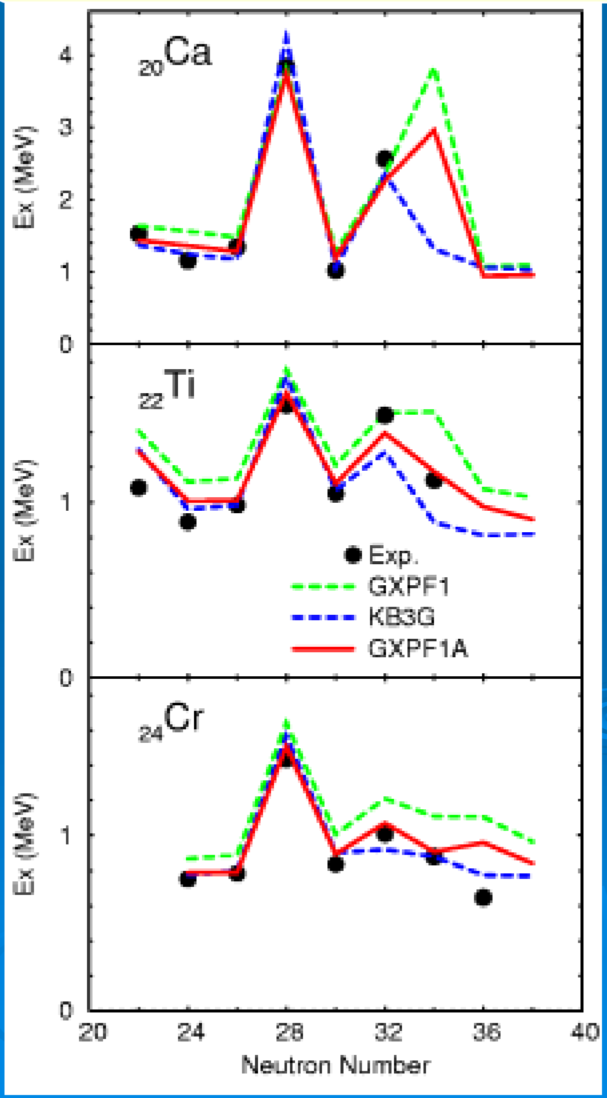
Diagonalization Shell Model

(medium-mass nuclei reached;dimensions 10^9!)

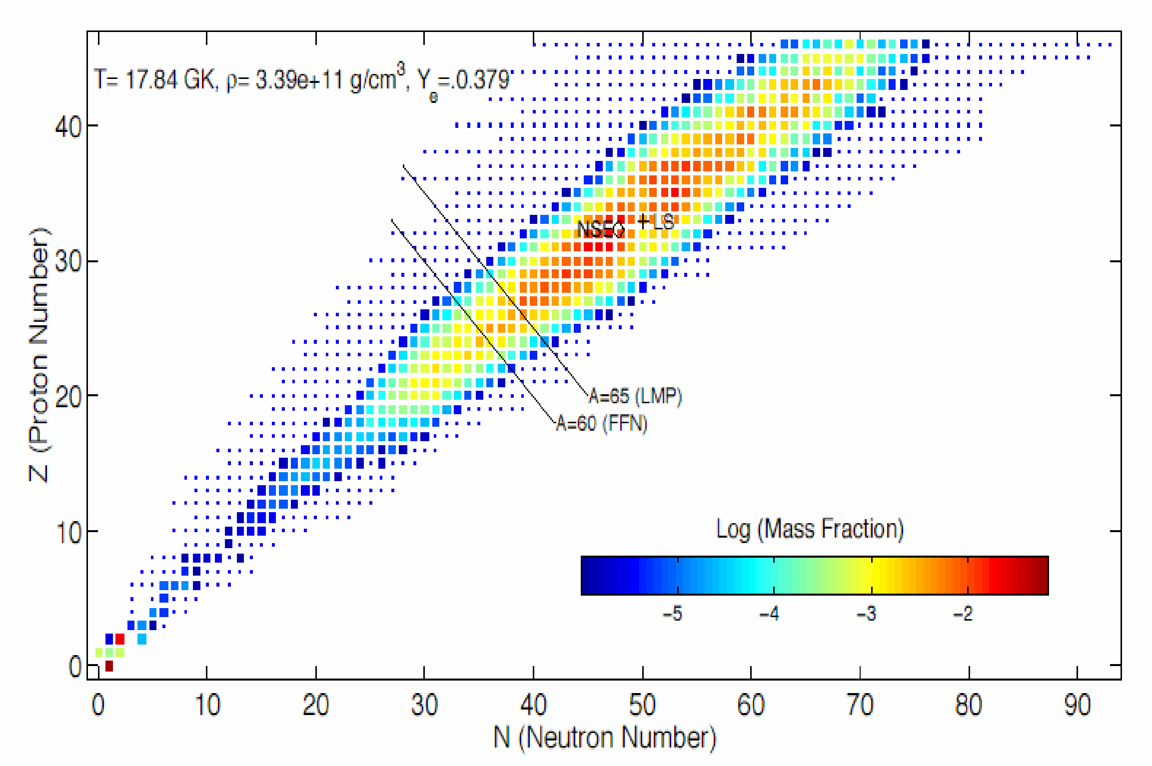


Martinez-Pinedo
ENAM'04

Honma, Otsuka et al., PRC69, 034335 (2004) and ENAM'04



Needed e$^-$ Capture Rates



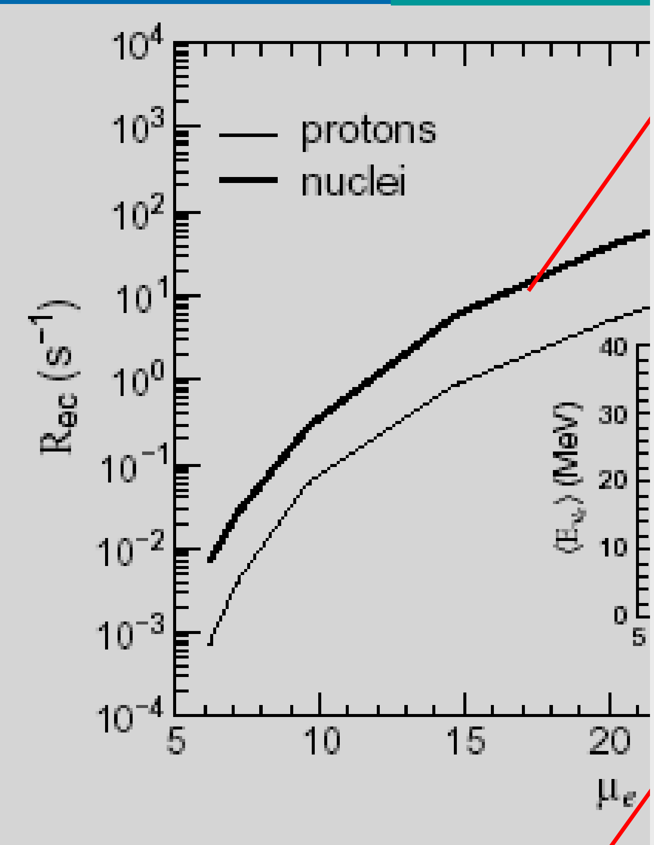
Need experimental BGT's in fp-gds shell nuclei. Experments being planned at MSU

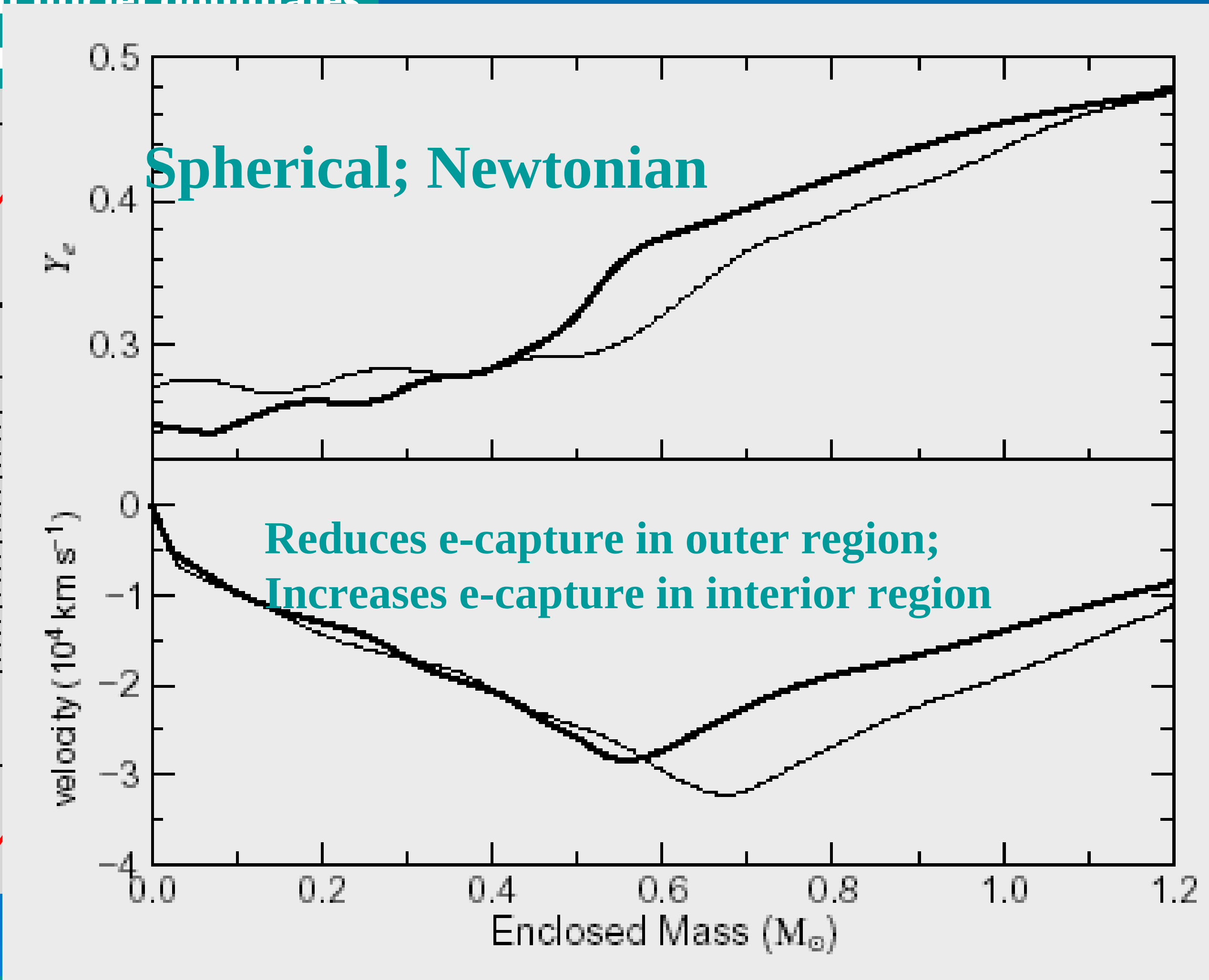
Nuclei with A>120 are present during collapse of the core.

See: Langanke, Martinez-Pinedo, Nucl. Phys. A673, 481 (2000)
Langanke, Kolbe, Dean, PRC63, 032801R (2001)
Langanke et al (PRL 2003) (rates calculation)
Hix et al (PRL, 2003) (core collapse implications)

Nuclear physics impact: changes in supernova dynamics

e-capture on nuclei dominates
e-capture o

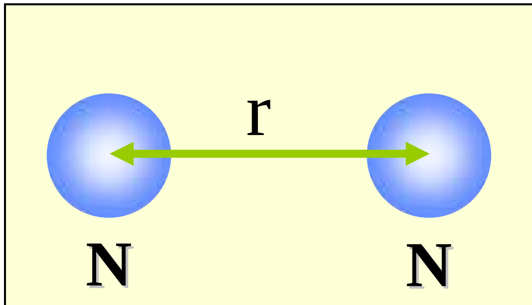




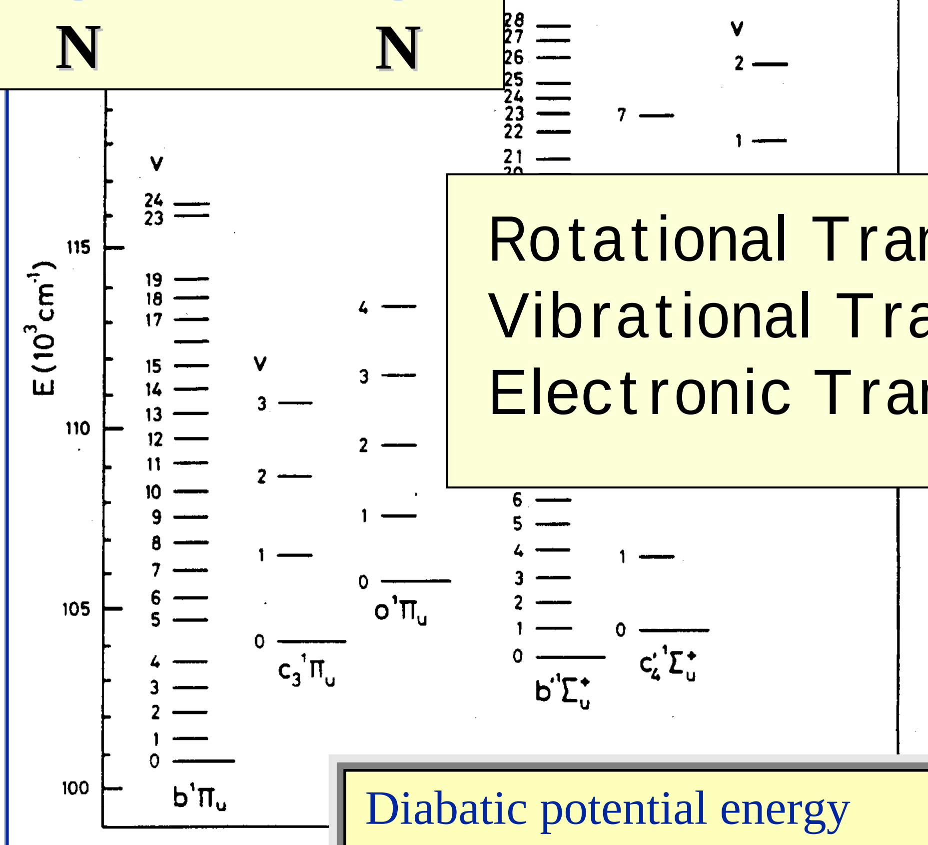
neutrino energies reduced

Shock forms deeper, is weaker,
but propagates farther before stalling

Scales: Excitation spectrum of N_2 molecule

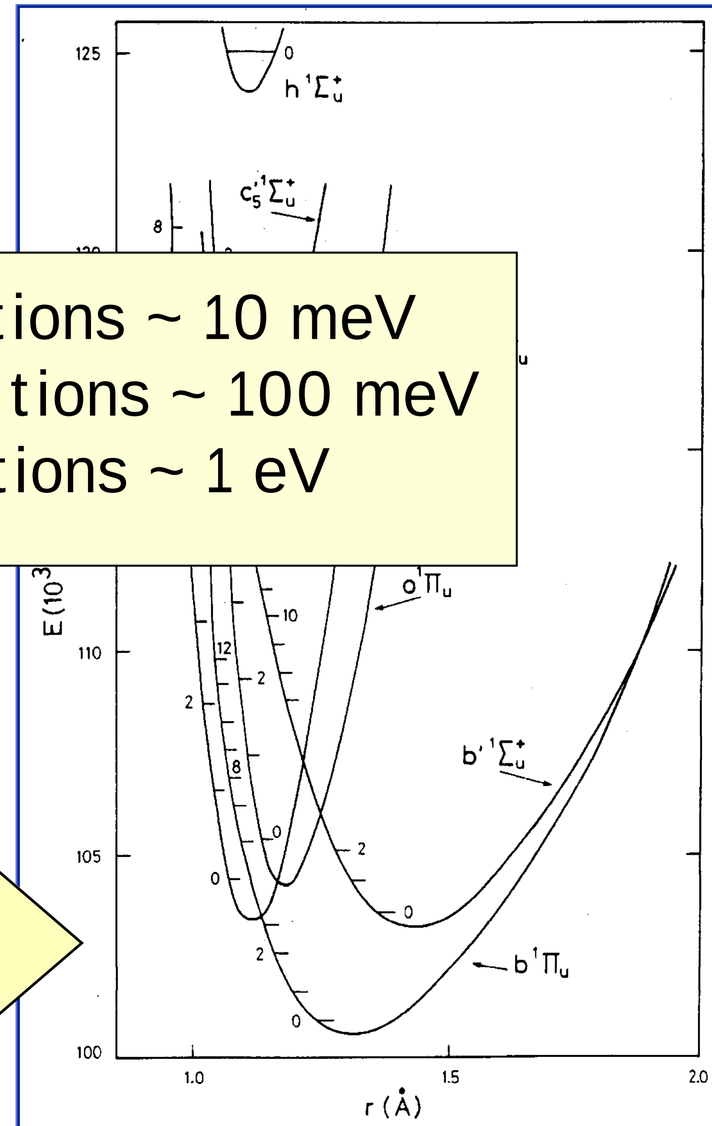


excited $^1\Sigma_u^+$ and $^1\Pi_u$ states

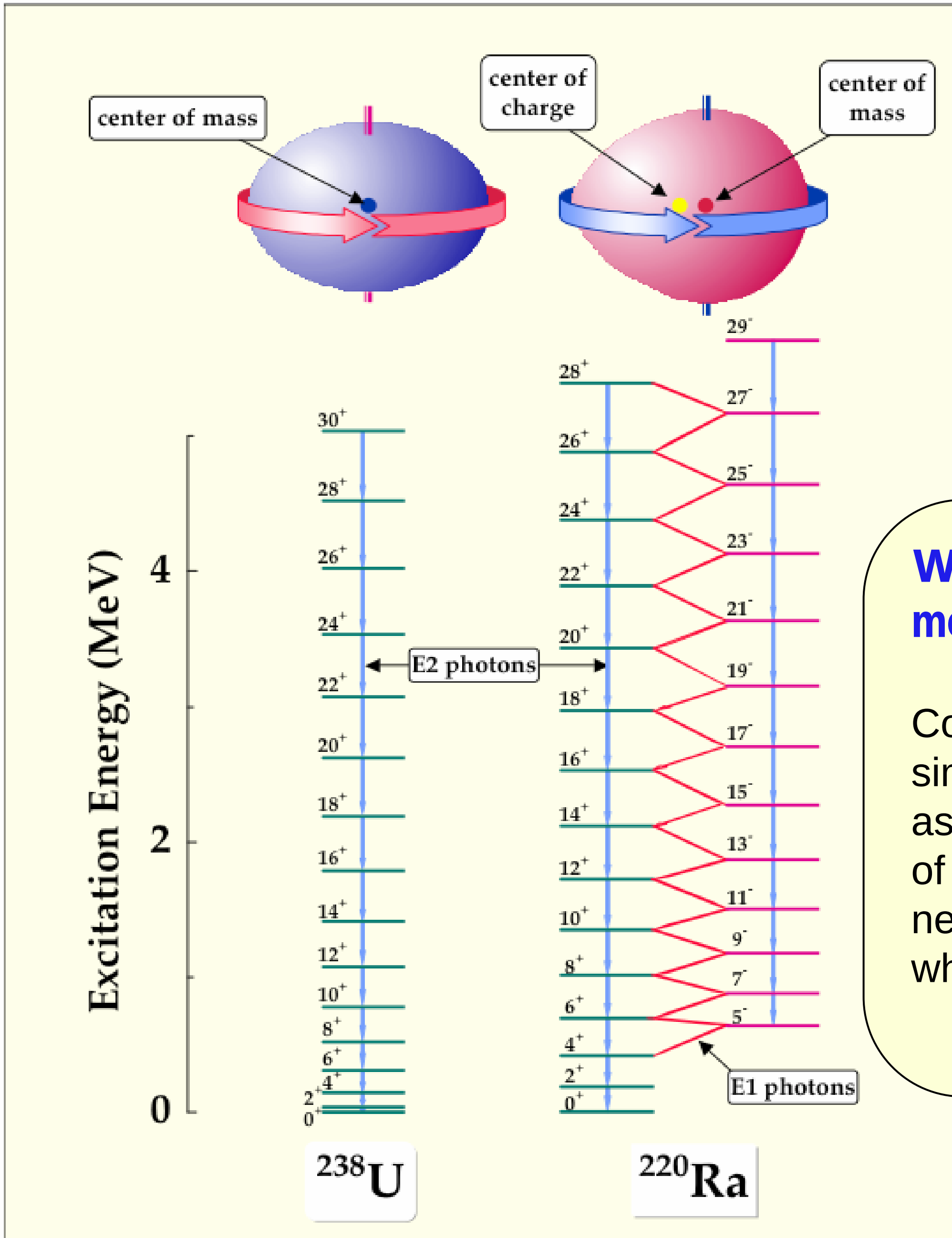


Rotational Transitions ~ 10 meV
Vibrational Transitions ~ 100 meV
Electronic Transitions ~ 1 eV

Diabatic potential energy surfaces for excited electronic configurations of N_2



Nuclear collective motion

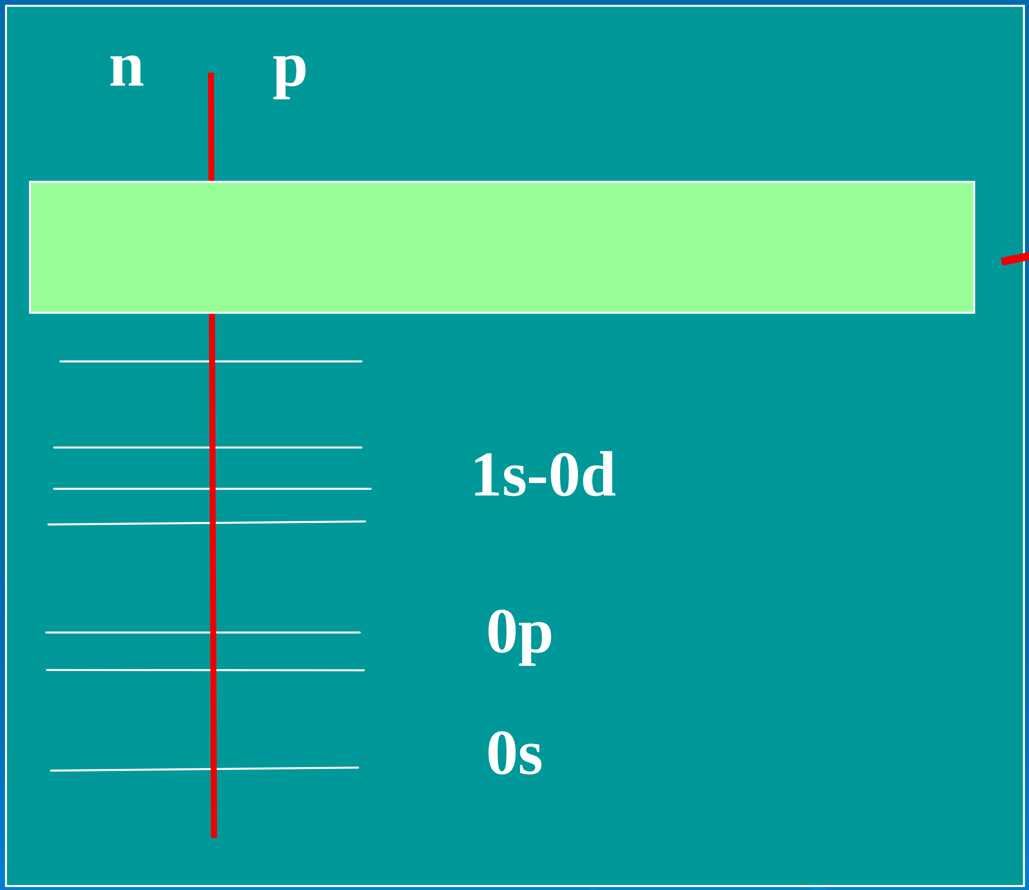


Rotational Transitions ~ 0.2-2 MeV
Vibrational Transitions ~ 0.5-12 MeV
Nucleonic Transitions ~ 7 MeV

What is the origin of ordered motion of complex nuclei?

Complex systems often display astonishing simplicities. Nuclei are no exception. It is astonishing that a heavy nucleus, consisting of hundreds of rapidly moving protons and neutrons can exhibit collective motion, where all particles slowly dance in unison.

Two basic approaches have been applied to ββ-decay problem (What are the masses of the neutrinos?)



1) Truncate the space to valance orbitals with an effective interaction (more correlations but less active orbitals)

2) Use a larger model space (more orbitals) but less correlations (RPA or QRPA – 1p-1h excitations)

Nuclear physics of the problem

$$T(0\nu)_{1/2}^{-1} = G_{0\nu}\left(\Delta E, Z\right)\left| M_{GT}^{0\nu} - \frac{g_V^2}{g_A^2} M_F^{0\nu} \right|^2 \left\langle m_\nu \right\rangle^2$$

$$M_F^{0\nu} = \left\langle f \left| \sum_{kj} H\left(r_{kj}, \overline{E}\right) \tau_k^+ \tau_j^+ \right| i \right\rangle$$

$$M_{GT}^{0\nu} = \left\langle f \left| \sum_{kj} H\left(r_{kj}, \overline{E}\right) \vec{\sigma}_k \cdot \vec{\sigma}_j \tau_k^+ \tau_j^+ \right| i \right\rangle$$

$$H\left(r, \overline{E}\right) = \frac{2R}{\pi r} \int_0^\infty dq \frac{q \sin qr}{\omega\left(\omega + E - \left[M_i + M_f\right]/2\right)}$$

Present published results

$$C_{mm} = \left[\langle m_\nu \rangle^2 T_{1/2}^{0\upsilon} / \right.$$

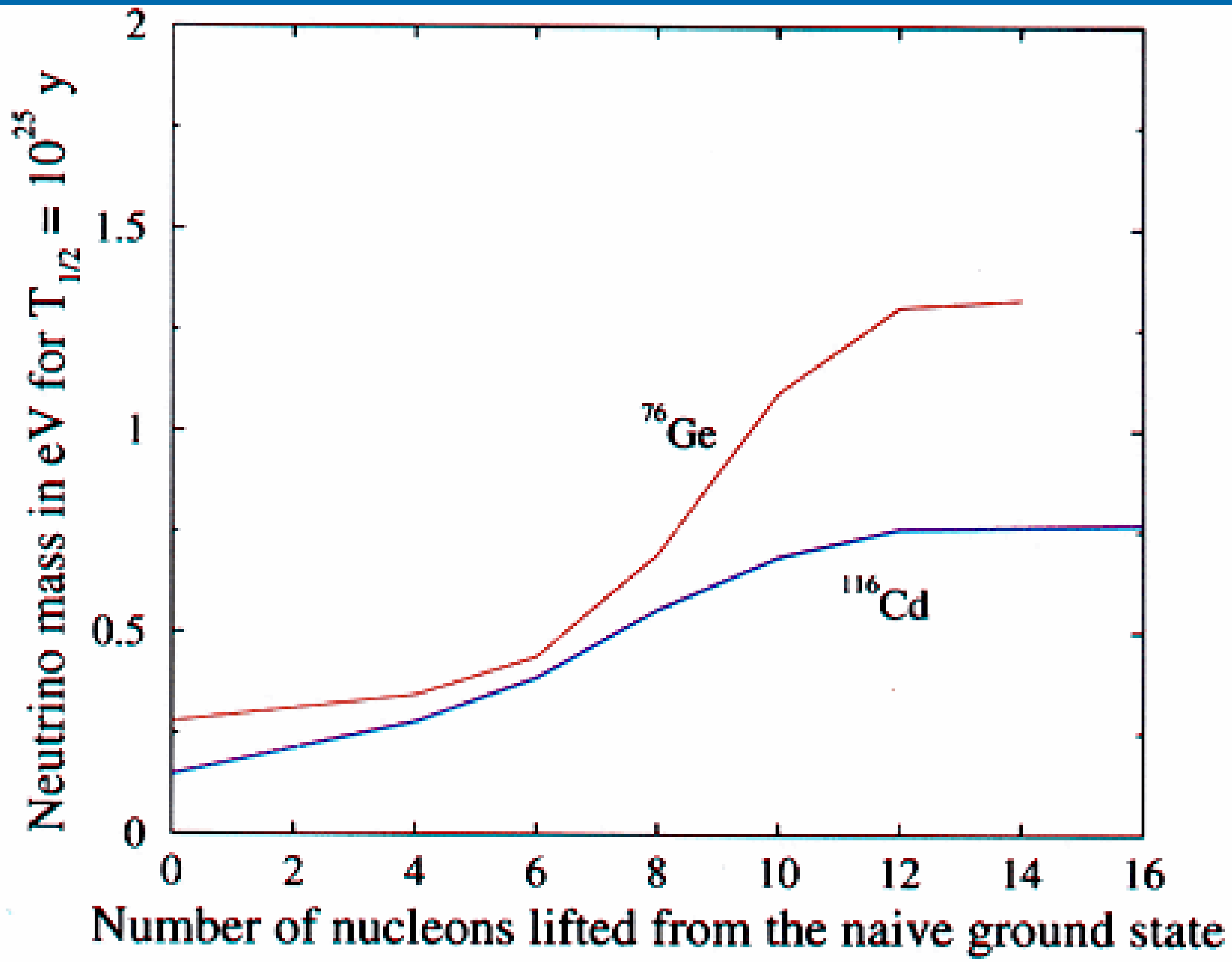
$C_{mm}(Y^{-1})$	$\langle m_\nu \rangle$ (eV)	Method	Reference
1.12×10^{-13}	0.024	QRPA	mut89,sta90[1, 2]
6.97×10^{-14}	0.031	QRPA	suh92[3]
7.51×10^{-13}	0.029	number-projected QRRA	suh92[3]
7.33×10^{-14}	0.030	QRPA	pan96[4]
1.18×10^{-13}	0.024	QRRA	tom91[5]
1.33×10^{-13}	0.022	QRPA	aun98[6]
8.27×10^{-14}	0.028	QRRA	bar99[7])
$1.85\text{-}12.5\times 10^{-14}$	0.059-0.023	QRPA	sto01a[8]
$1.8\text{-}2.2\times 10^{-14}$	0.060-0.054	QRRA	bob01[9]
6.9970959×10^{-14}	0.031	QRPA	civ03[10]
1.42×10^{-14}	0.068	QRRA with np pairing	pan96[4])
4.53×10^{-14}	0.038	QRPA with forbidden	rod03[11]
8.29×10^{-14}	0.028	RQRPA	fae98[12]
1.03×10^{-13}	0.025	RQRRA	sim99[13]
6.19×10^{-14}	0.032	RQRRA with forbidden	sim99[13]
$5.5\text{-}6.3\times 10^{-14}$	0.034-0.032	RQRRA	bob01[9]
$2.21\text{-}8.83\times 10^{-14}$	0.054-0.027	RQRPA	sto01a[8]
3.63×10^{-14}	0.042	RQRPA with forbidden	rod03[11]
2.75×10^{-14}	0.049	Full RQRPA	sim97[14]
$3.36\text{-}8.54\times 10^{-14}$	0.042-0.028	Full RQRPA	sto01a[8]
$6.50\text{-}9.21\times 10^{-14}$	0.032-0.027	Second QRPA	sto01a[8]
$2.7\text{-}3.2\times 10^{-15}$	0.155-143	Self-consistent QRA	bob01[9]
2.88×10^{-13}	0.015	VAMPIR	tom86[15]
1.58×10^{-13}	0.020	Shell-model truncation	hax84[16]
$6.87\text{-}15.7\times 10^{-14}$	0.031-0.020	Shell-model truncation	eng89[17]
1.90×10^{-14}	0.059	Large-scale shell model	cau96[18]

Kill outliers

Factor of 3 in C_{mm}

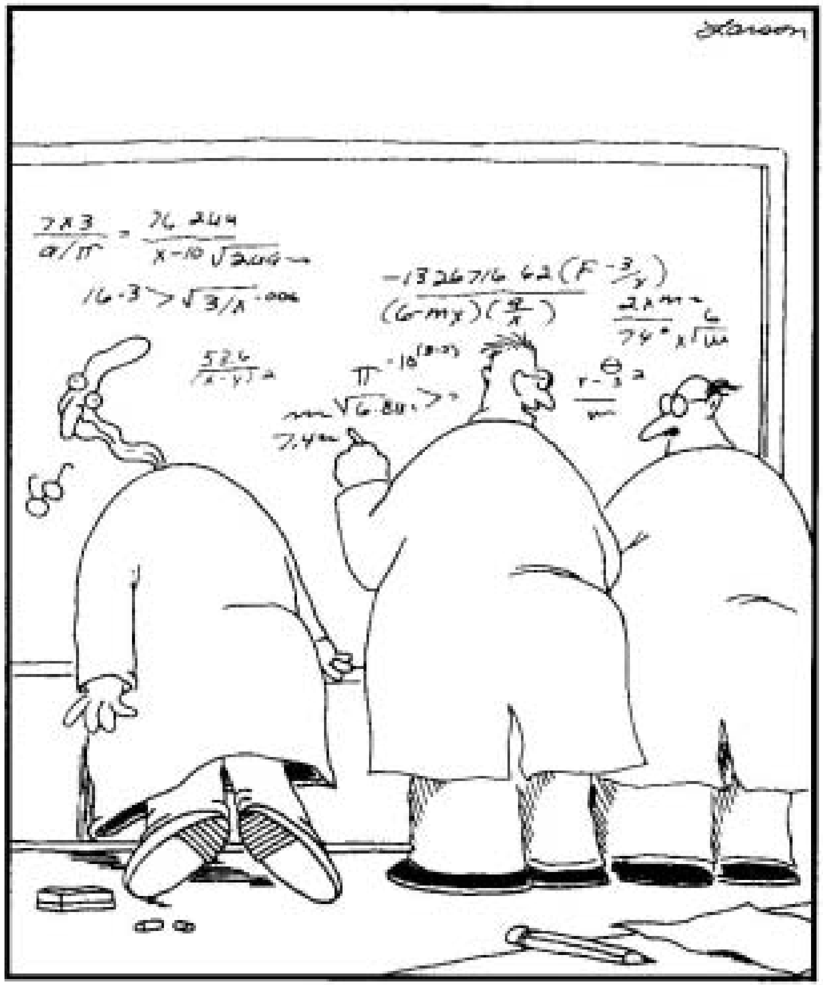
Assume T1/2 =4E-27 years

What the shell-model calculations predict



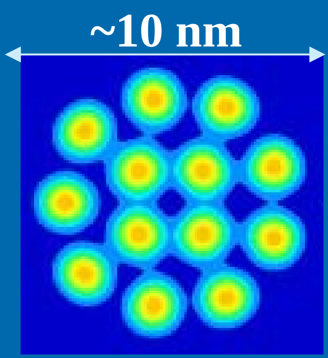
Caurier et al

So now, we have to start doing some theory…

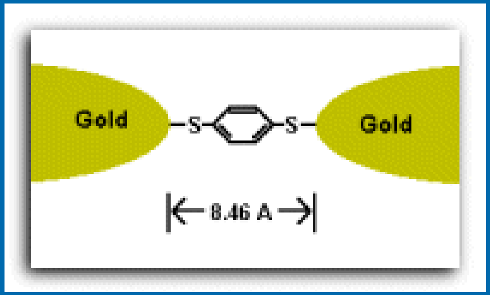


"Ha! Webster's blown his cerebral cortex."

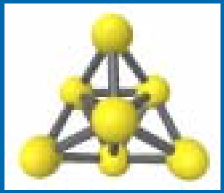
Before we worry about nuclei: a very general look at quantum many-body problems

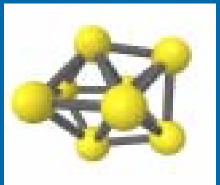


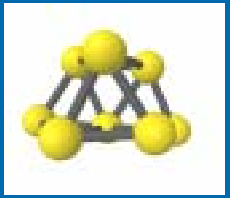
2-d quantum dot
strong magnetic field
localization

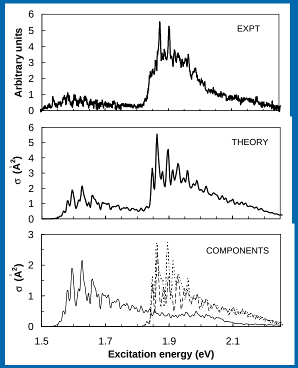


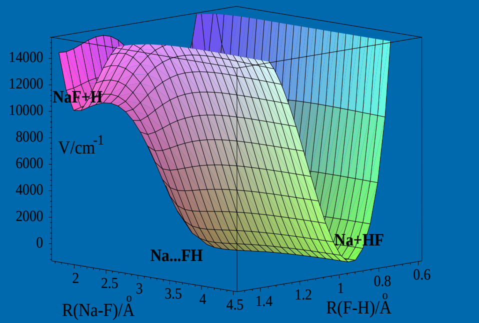
Molecular scale:
conductance
delocalized orbitals











Chemical reaction pathways

Quantum mechanics plays a role when the size of the object is of the same order as the interaction length.

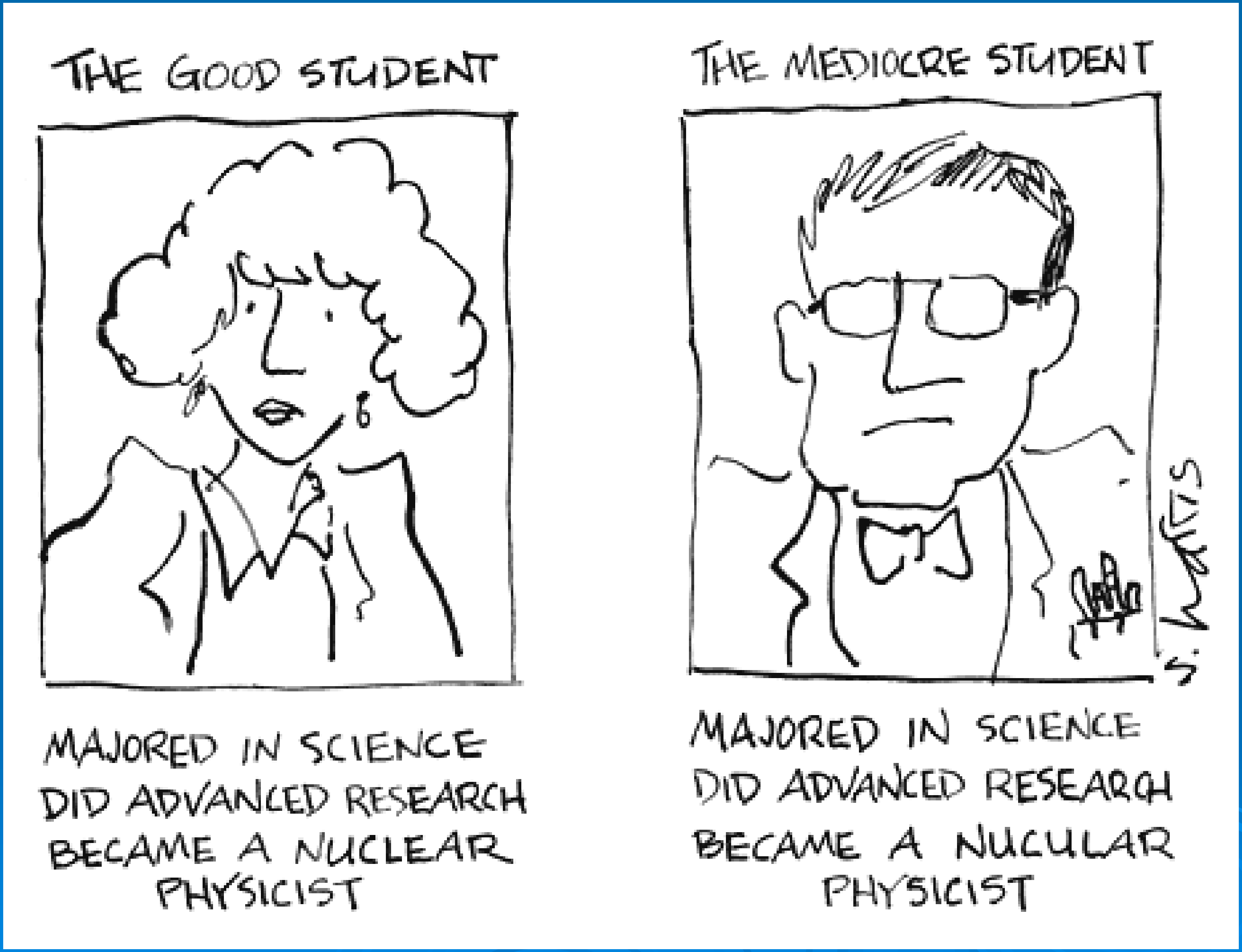
Common properties

- Shell structure
- Excitation modes
- Correlations
- *Phase transitions*
- Interactions with external probes

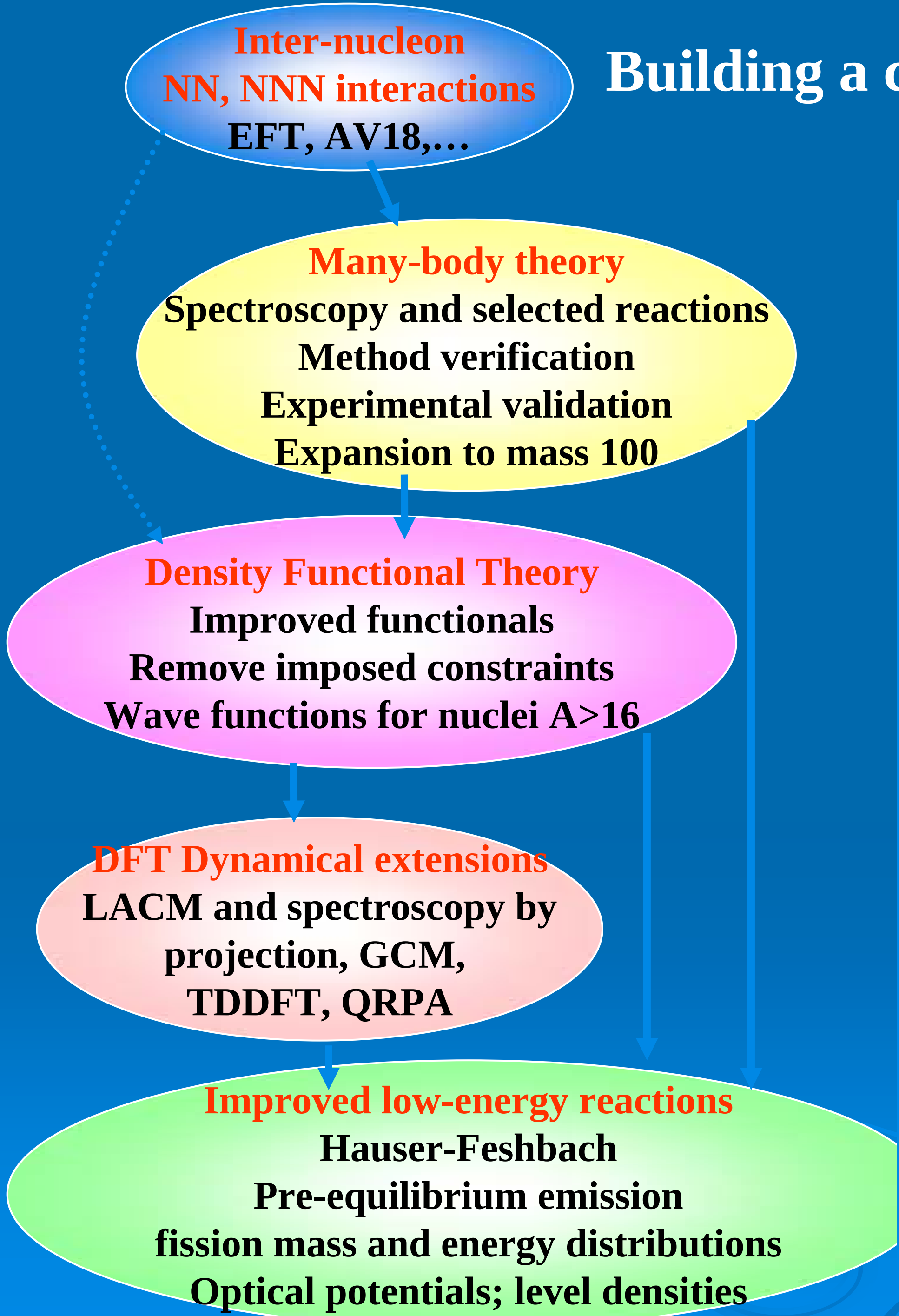
Quantum many-body problems

I. Solving the many-body problem
II. The nuclear interaction
III. ab initio in light nuclei
IV. Nuclear Density Functional Theory

I hope you are all good students



Building a coherent theoretical path forward



RIA Theory Blue Book (2005)

Theoretical challenges must be met during the next decade in order to facilitate the success of an experimental program focused on short-lived isotopes and to enhance the national effort in nuclear science.

These efforts include:

• Development of ab initio approaches to medium-mass nuclei

• Development of self-consistent nuclear density-functional theory methods for static and dynamic problems.

• Development of reaction theory that incorporates relevant degrees of freedom for weakly bound nuclei.

• Exploration of isospin degrees of freedom of the density-dependence of the effective interaction in nuclei.

• Development and synthesis of nuclear theory, and its consequent predictions, into various astrophysical models to determine the nucleosynthesis in stars.

• Development of robust theory and error analysis for nuclear reactions relevant to NNSA and GNEP

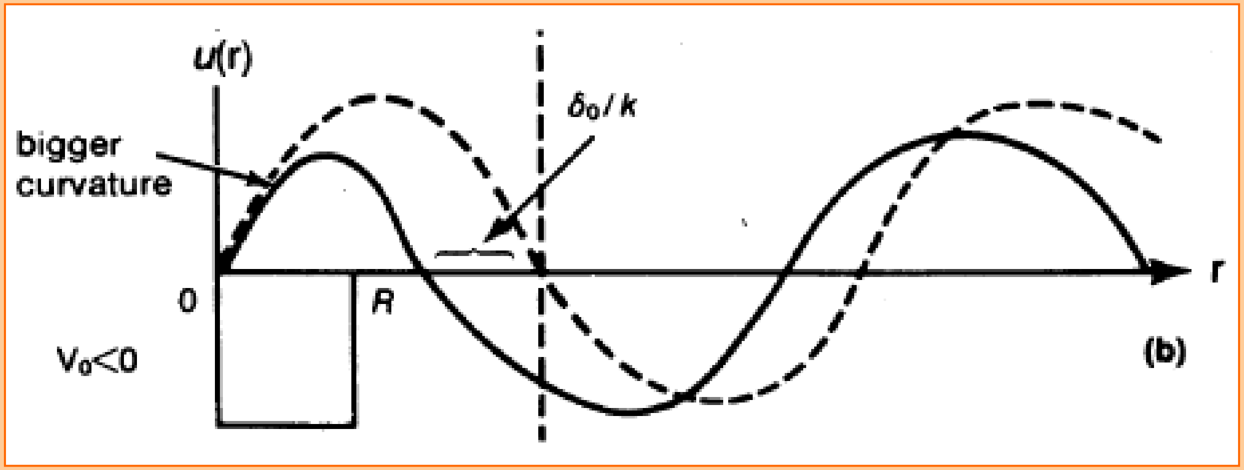
The Nucleon-Nucleon interaction

- Deuteron with $J^{\pi}=1^{+}$ → attraction at least in the $^3S_1$ partial wave
- Interference between Coulomb and nuclear scattering for proton-prton partial wave $^1S_0$ → attractive NN force at least in the $^1S_0$ channel
- NN force has a short range
- Different scattering lengths for triplet and singlet states → spin dependence
- Observation of large polarization of scattered nucleons perpendicular to the plane of scattering → spin-orbit force
- s-wave phase shift becomes negative at ~250 MeV → Hard core with range of 0.4-0.5 fm
- Charge independence (almost) → Charge symmetry breaking (CSB)
- Two nucleons in a given two-body state (almost) feel the same force → charge independence breaking (CIB)
- Quadrupole moment of the deuteron points to an admixture of both l=2 ($^3D_1$) and l=0 ($^3S_1$) orbital momenta → tensor force

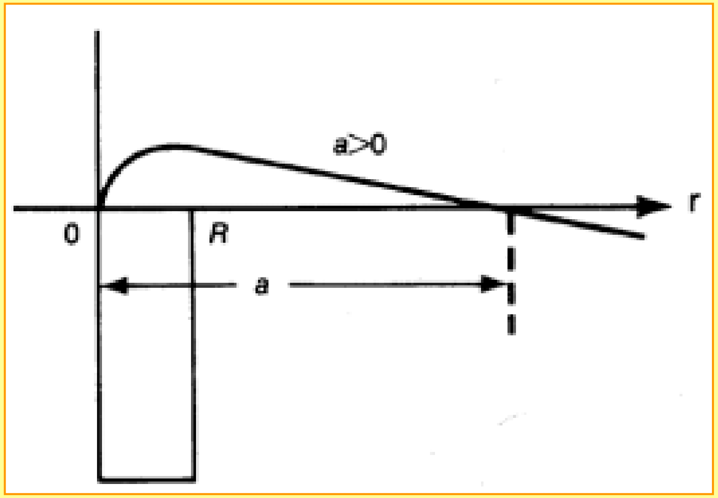
$$O_{ij}^{p=1,14} = 1, \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j, \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j, (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), S_{ij}, S_{ij}(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), \mathbf{L}\cdot\mathbf{S}, \mathbf{L}\cdot\mathbf{S}(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), \\ L^2, L^2(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), L^2(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j), L^2(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), (\mathbf{L}\cdot\mathbf{S})^2, (\mathbf{L}\cdot\mathbf{S})^2(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)$$

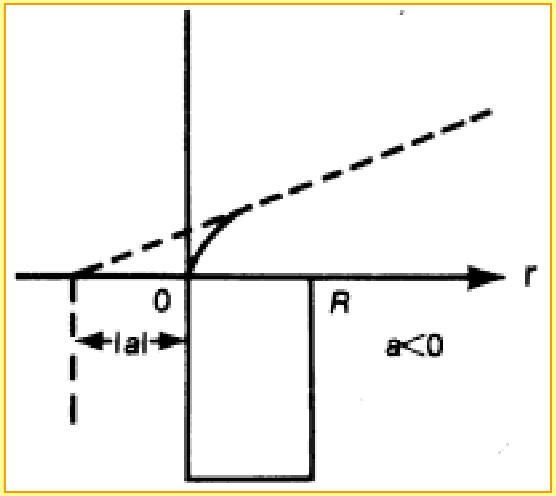
Recapitulation: Scattering theory

Phase shift Ω(k) is a function of relative momentum k; Figure shows s-wave.



Scattering length: $k \cot \delta(k) \approx -\frac{1}{a}; \quad \sigma_{tot} \approx 4\pi a^2 \quad \text{for} \quad k \to 0$

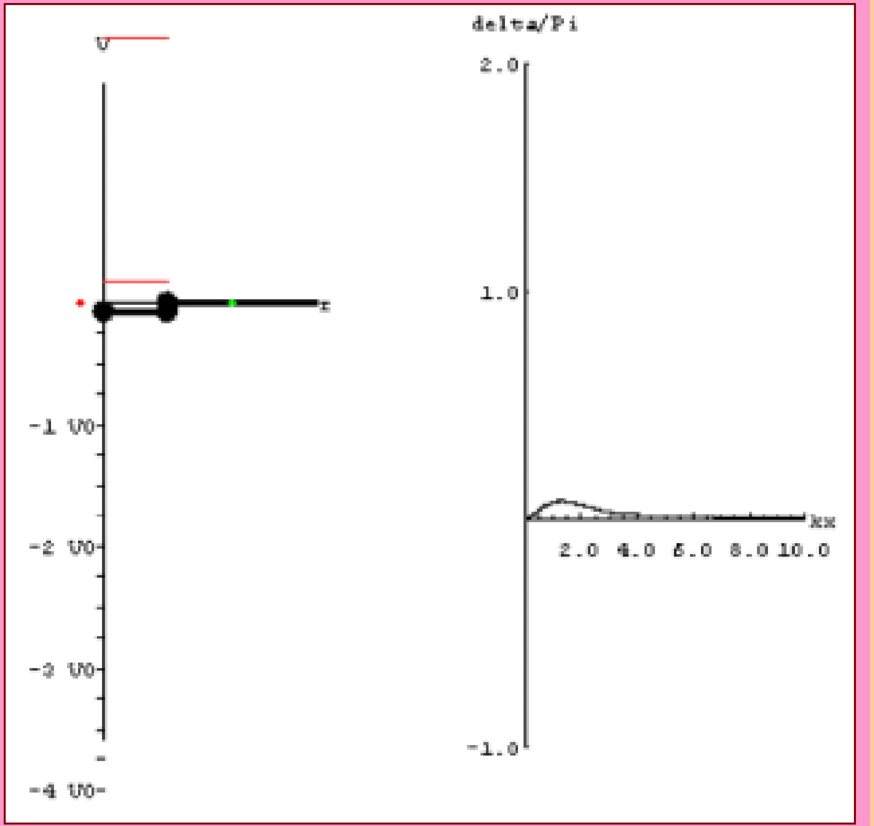




Scattering from a spherical well

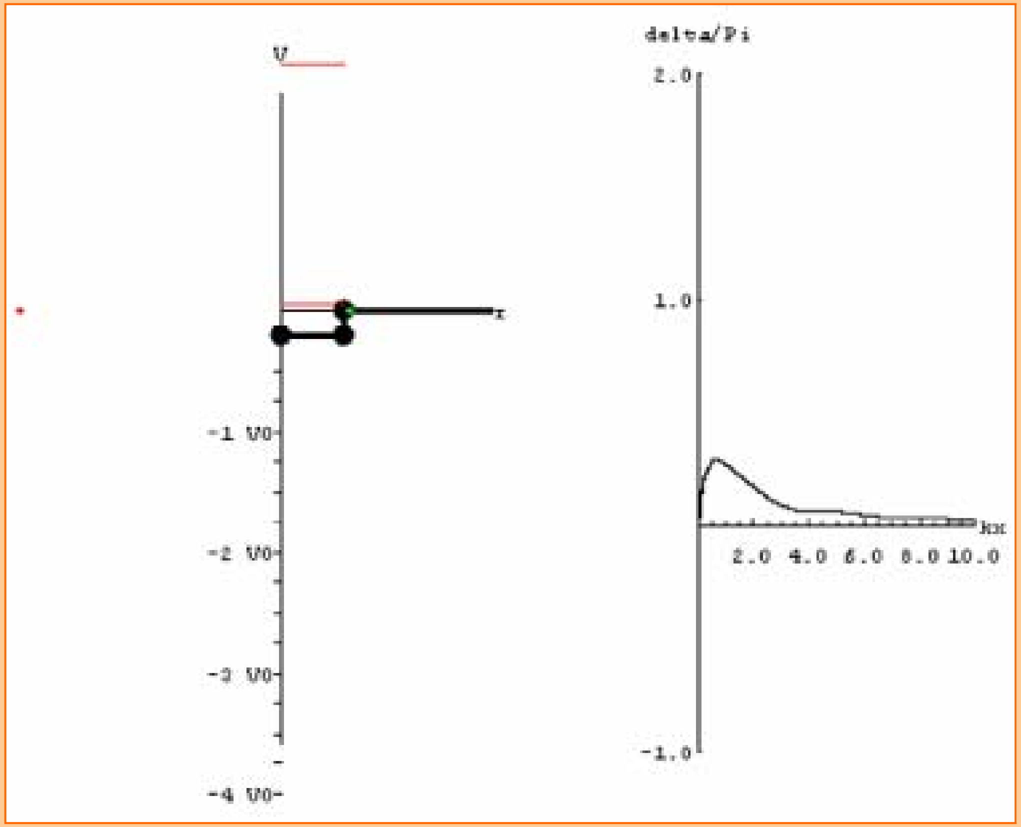
http://people.ccmr.cornell.edu/~emueller/scatter/well.html

System has no bound state



Increase depth of well:

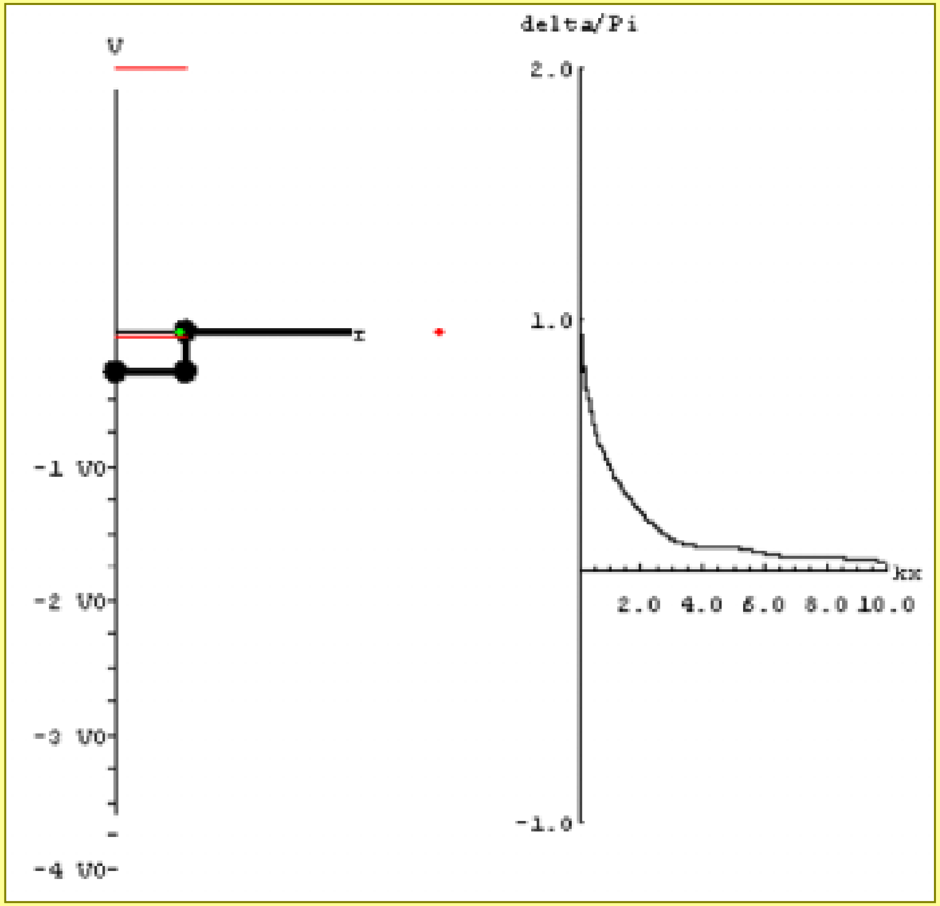
First bound state is about to enter



Scattering from a spherical well

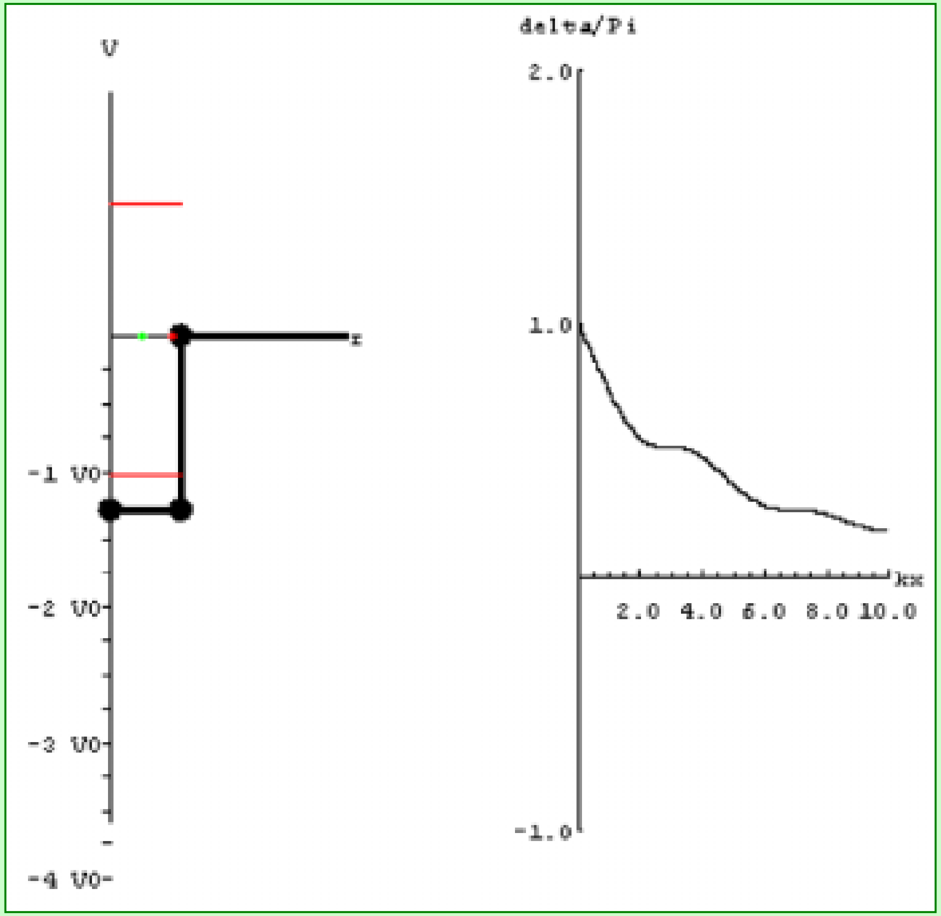
Further increase of depth:

System has one shallow bound state



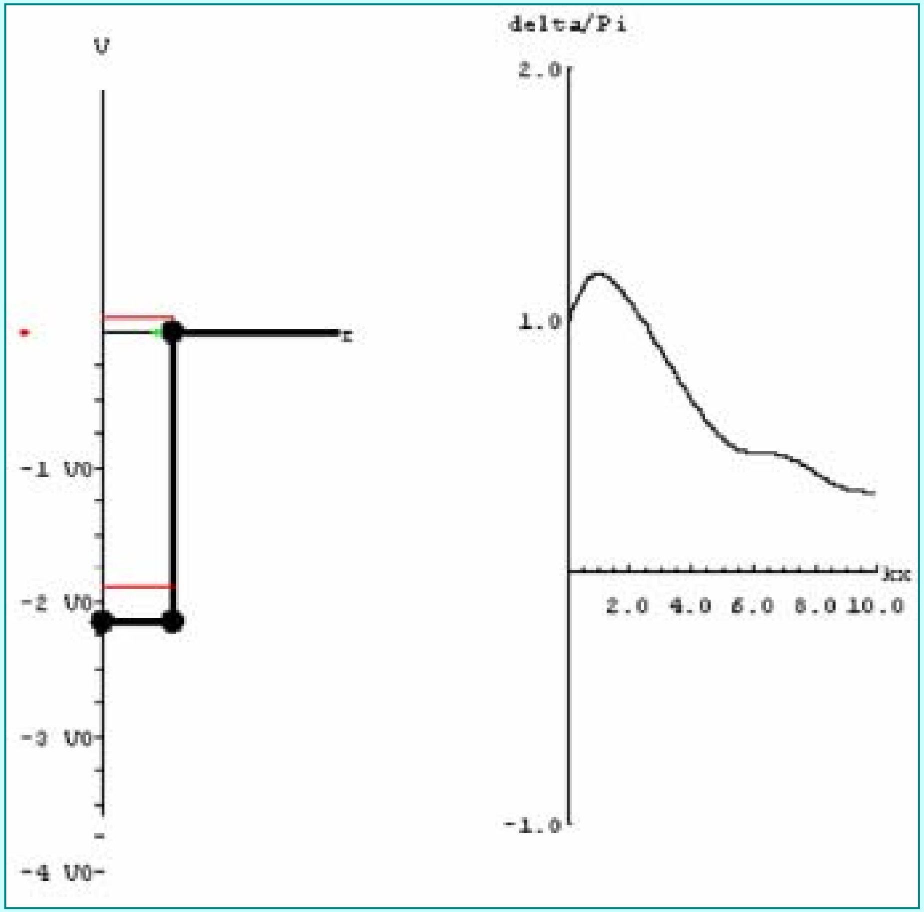
Further increase of depth:

System has one deep bound state

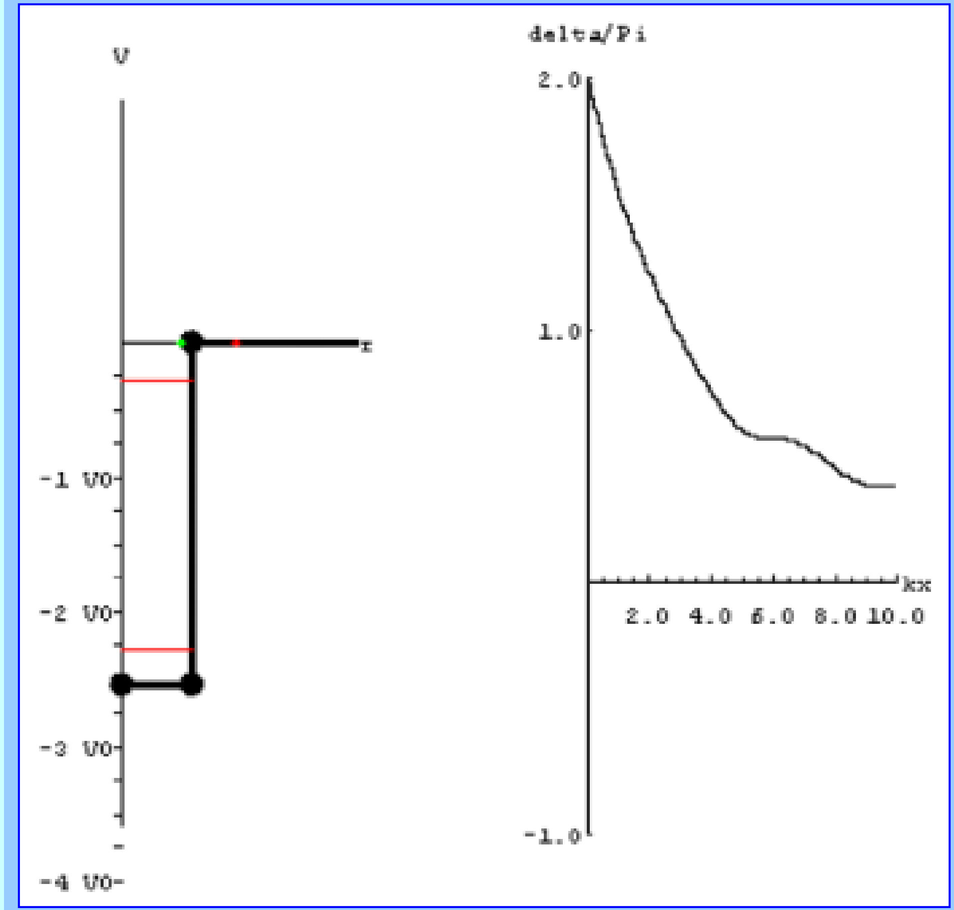


Scattering from a spherical well

Second bound state about to enter

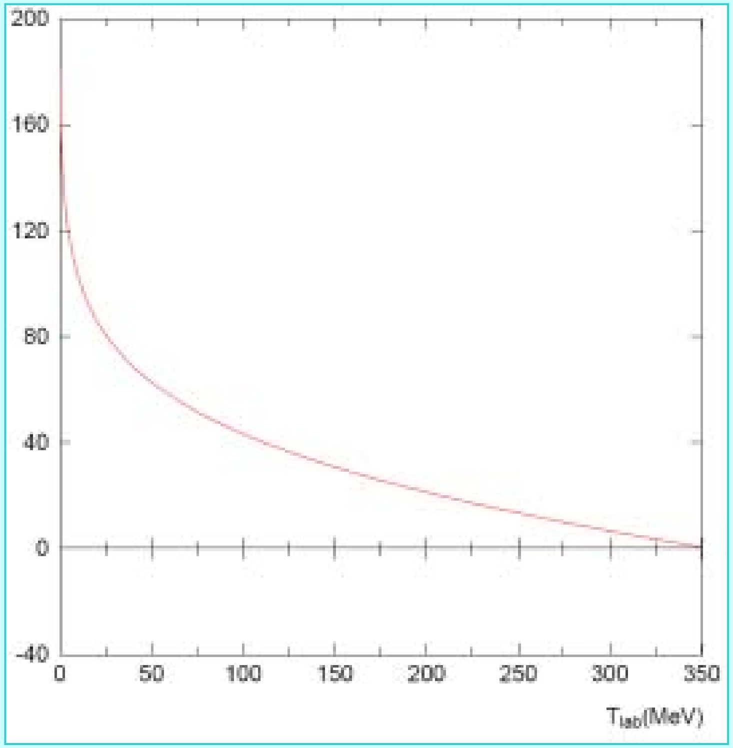


System has two bound state



Nuclear s-wave phase shifts

http://nn-online.org/

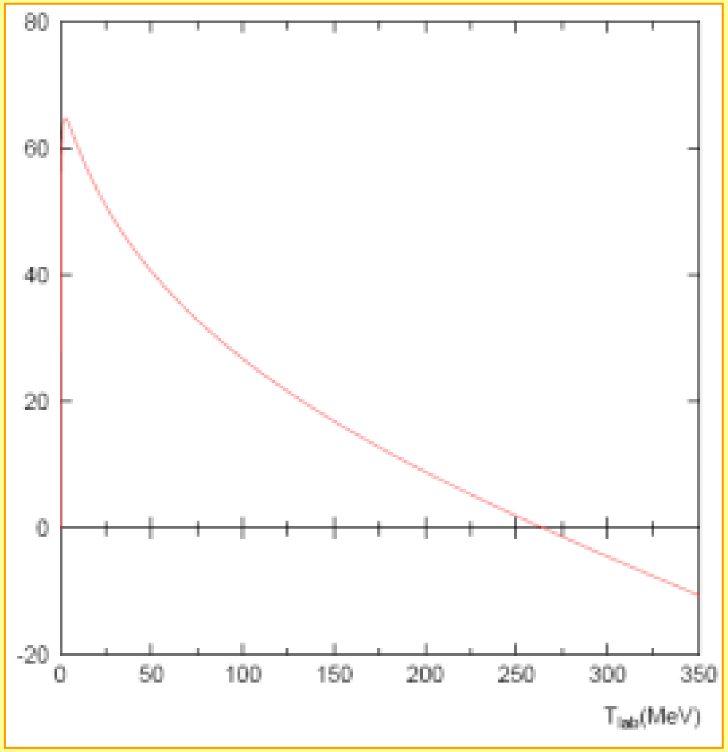


Deuteron is a very weakly bound system!

System has one bound state.

Steep decrease from 180 degrees due to large scattering length.

Acts repulsive due to large (positive) scattering length.



System (barely) fails to exhibit bound state.

Steep rise at 0 due to large scattering length.

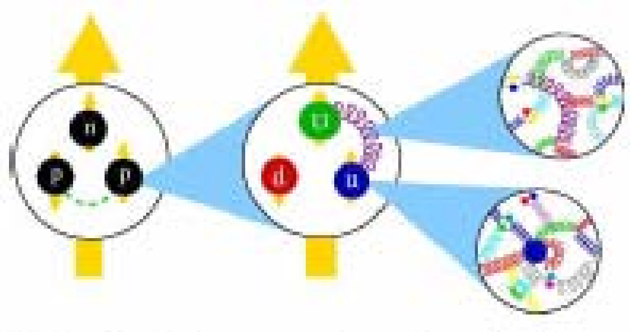
Monotonous decrease due to hard core.

A (very) brief history of NN interactions

1935 – Yukawa (meson theory)
1957 – Gammel and Thaler (full theory of OPE)
1960’s – non-relativistic OBEP (pions, scalar mesons)
Bryan-Scott potential (1969)
1970’s – fully relativistic OBEPs
-- 2-pion exchange
1980’s – Nijmegen potentials (1978)
1990’s – Nijmegan II, Bonn potentials
1990’s – AV18 + 3body potentials
2000’s – EFT potentials (2 and 3 body)

χ^2/dof = 10 in 1960’s ; = 2 in 1980’s ; = 1 in 1990’s….

Effective Field Theory



Interplay between nucleonic and sub-nucleonic (quarks and gluons) degrees of freedom in few-body nuclear systems

It's pretty complicated inside a nucleon!!

Starting point is an effective chiral πN Lagrangian:

$$L_{\pi N} = L_{\pi N}^{(1)} + L_{\pi N}^{(2)} + L_{\pi N}^{(3)} + \cdots$$

- Obeys QCD symmetries (spin, isospin, chiral symmetry)
- Develops a low-momentum interaction suitable for nuclei
- ?Should some day be connected directly to QCD?

$$L_{\pi N}^{(1)} = \overline{N}\left(iD_0 - \frac{g_A}{2}\vec{\sigma}\bullet\vec{u} \right)N \approx \overline{N}\left[i\partial_0 - \frac{1}{4f_\pi^2}\tau\bullet(\pi\times\partial_0\pi) - \frac{g_A}{2f_\pi}\tau\bullet(\vec{\sigma}\bullet\nabla)\pi \right]N + \cdots$$

Chiral Perturbation theory

"If you want more accuracy, you have to use more theory (more orders)"

Effective Lagrangian → obeys QCD symmetries (spin, isospin, chiral [illegible] symmetry breaking)

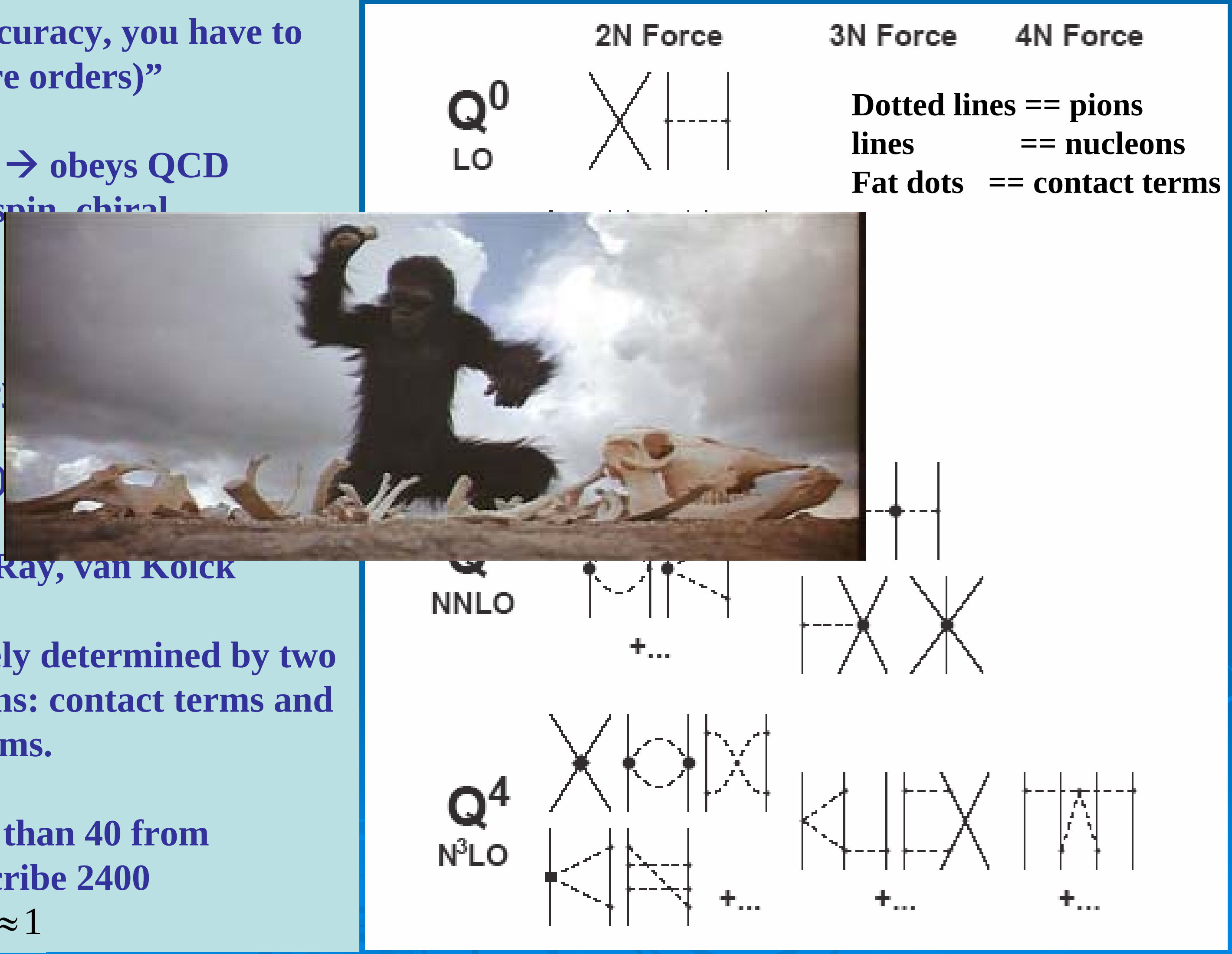
Lagrangian
→ infinite sum of Fe[illegible]

Expand in $O(Q/\Lambda_{QCD})$[illegible]

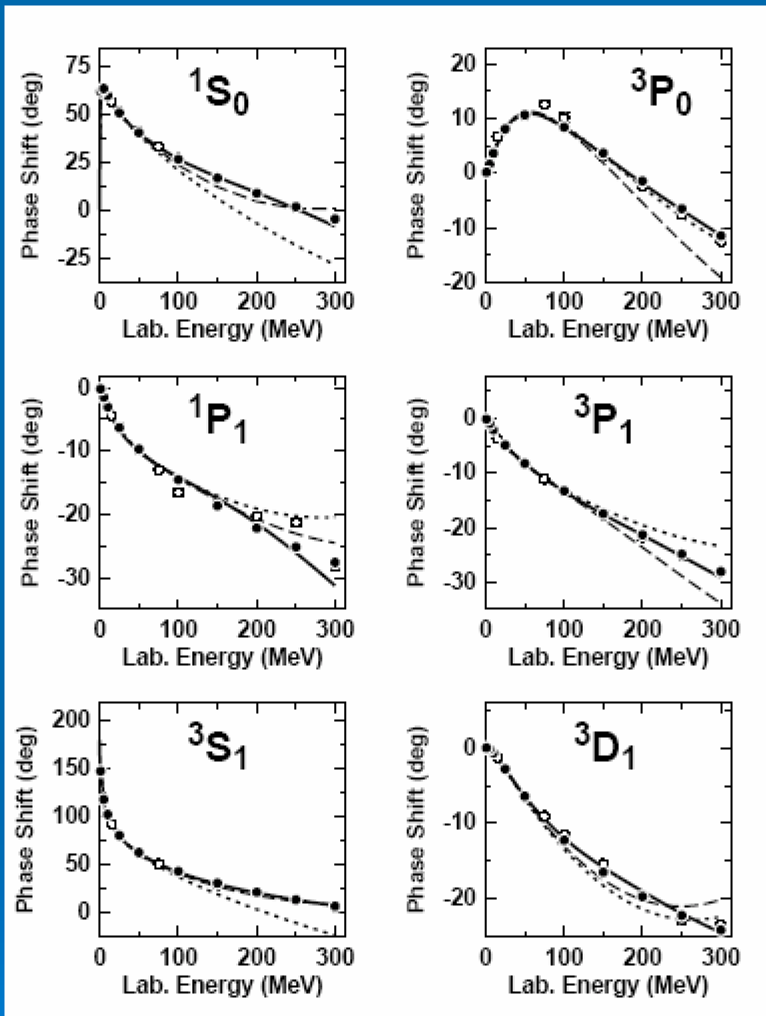
Weinberg, Ordonez, Ray, van Kolck

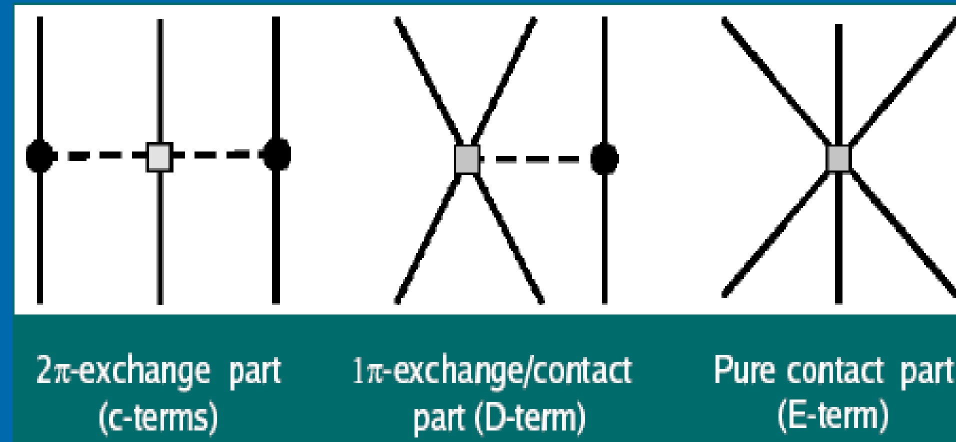
NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

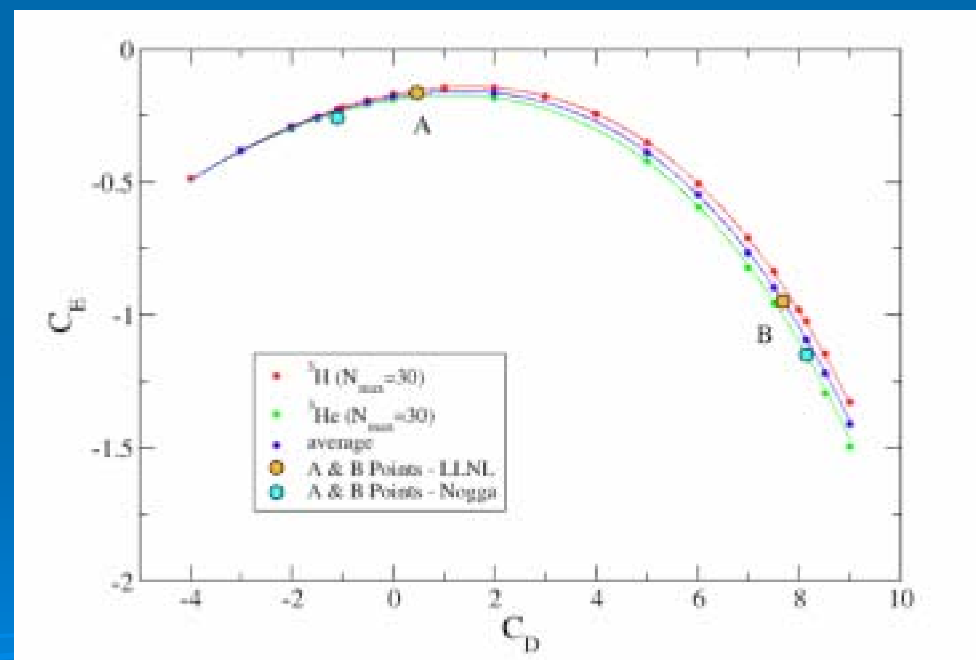
24 paramters (rather than 40 from meson theory) to describe 2400 data points with $\chi^2_{\text{dof}} \approx 1$



Effective field theory potentials bring a 3-body force







Challenge: Deliver the best NN and NNN interactions with their roots in QCD.

Translating scattering matrix to potential: Lippmann-Schwinger

- There is a covariant formulation (heuristic and equal times shown below)

$$(H_0 + V)|\psi_k\rangle = k^2|\psi_k\rangle \quad (H_0 - k^2)|\varphi_k\rangle = 0$$

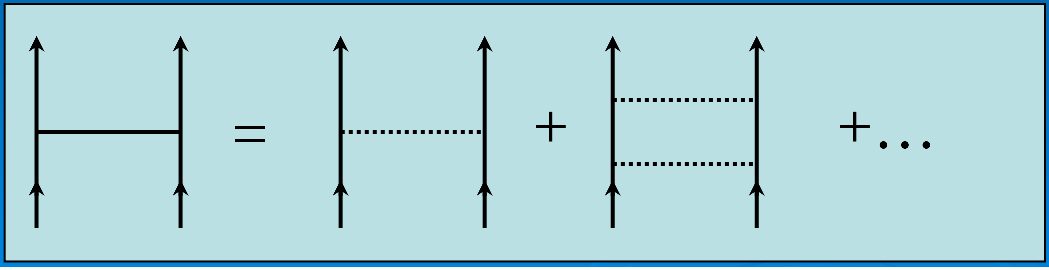
$$|\psi_k\rangle = |\varphi_k\rangle + G(E_k)V|\psi_k\rangle \quad G(E_k) = \frac{1}{E_k - H_0 + i\varepsilon}$$

outgoing b.c.

$$V|\psi_k\rangle = V|\varphi_k\rangle + VG(E_k)V|\psi_k\rangle$$

$$T(E_k)|\varphi_k\rangle = V|\psi_k\rangle$$

$$T(E_k) = V + VG(E_k)T(E_k)$$



$$O_{ij}^{p=1,14} = 1, \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j, \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j, (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), S_{ij}, S_{ij}(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), \mathbf{L}\cdot\mathbf{S}, \mathbf{L}\cdot\mathbf{S}(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), L^2, L^2(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), L^2(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j), L^2(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), (\mathbf{L}\cdot\mathbf{S})^2, (\mathbf{L}\cdot\mathbf{S})^2(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)$$

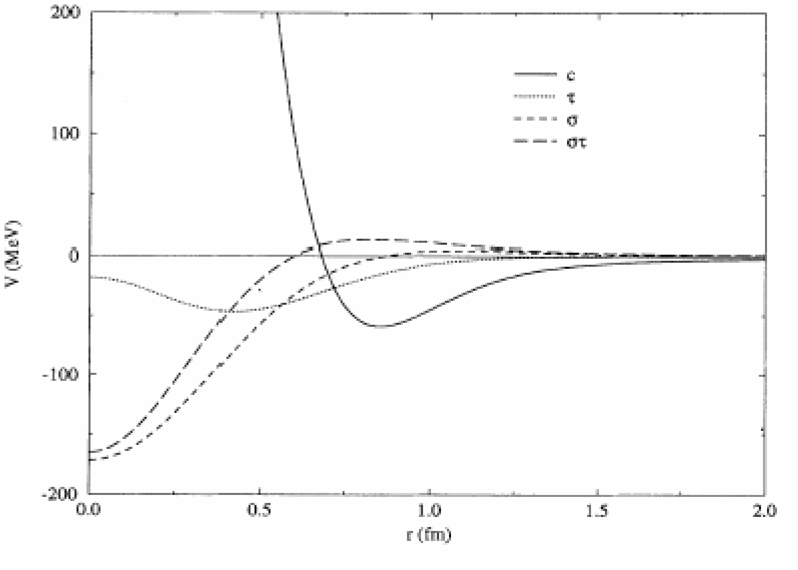


FIG. 6. Central, isospin, spin, and spin-isospin components

Challenge: Explosion of the basis calls for different approaches!

Begin with a bare NN (+3N) Hamiltonian

$$H = -\frac{\hbar}{2}\sum_{i=1}^{A}\frac{\nabla_i^2}{m_i} + \frac{1}{2}\sum_{i<j} V_{2N}\left(\vec{r}_i,\vec{r}_j\right) + \frac{1}{6}\sum_{i<j<k} V_{3N}\left(\vec{r}_i,\vec{r}_j,\vec{r}_k\right)$$

→ **Bare (GFMC)**

→ **Basis expansion**

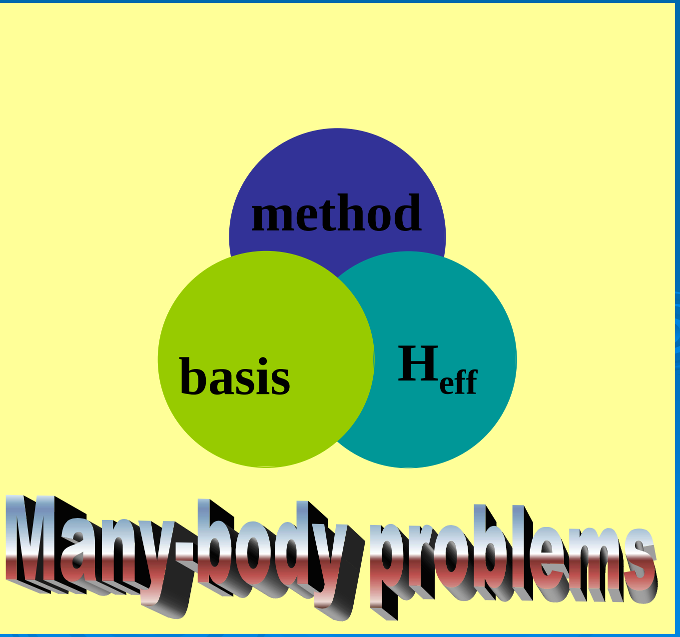
Basis expansions:

- Choose the method of solution
- Determine the appropriate basis
- Generate H_{eff}

Nucleus	4 shells	7 shells
4He	4E4	9E6
8B	4E8	5E13
12C	6E11	4E19
16O	3E14	9E24

Oscillator single-particle basis states

Many-body basis states



Green's Function Monte Carlo

Idea:

1. **Determine accurate approximate wave function via variation of the energy (The high-dimensional integrals are done via Monte Carlo integration).**

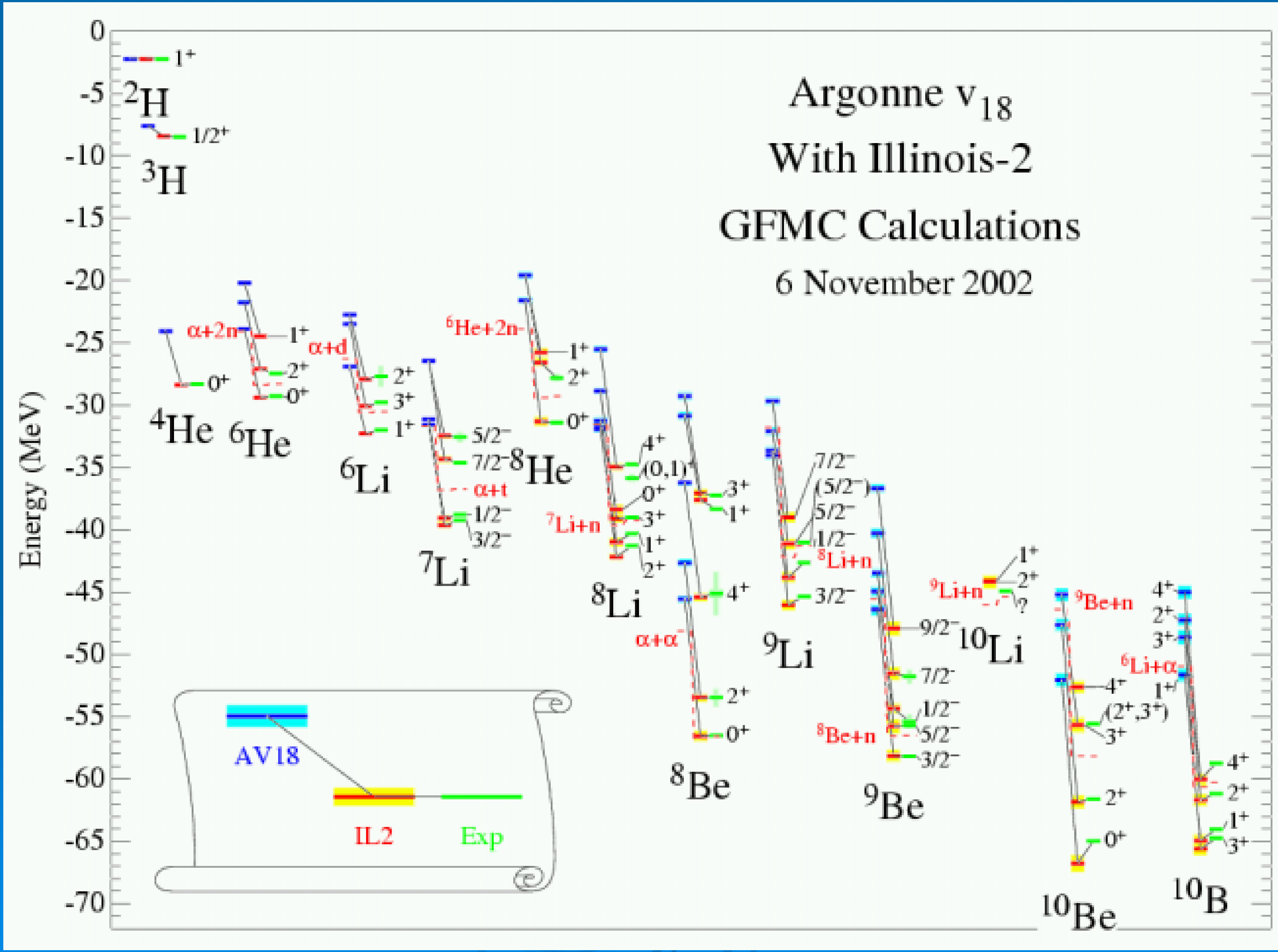
$$E = \frac{\langle \Psi_{\text{trial}} | \hat{H} | \Psi_{\text{trial}} \rangle}{\langle \Psi_{\text{trial}} | \Psi_{\text{trial}} \rangle}$$

2. **Refine wave function and energy via projection with Green's function**

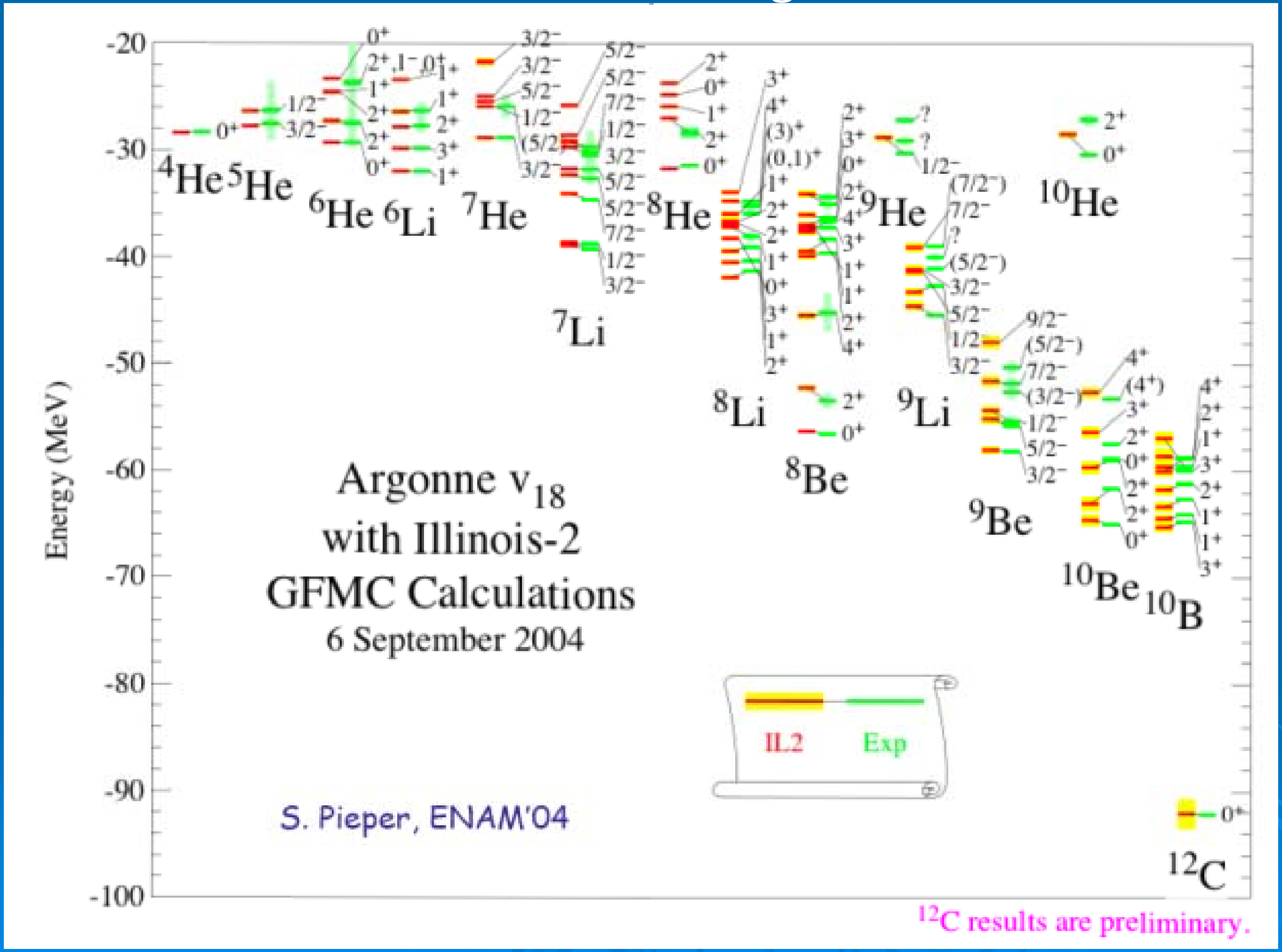
$$|\Psi\rangle = \lim_{\tau \to \infty} e^{-\tau(\hat{H}-E)} |\Psi_{\text{trial}}\rangle$$

- ☺ **Virtually exact method.**
- ☹ **Limited to certain forms of Hamiltonians.**
- ☹ **Computational expense increases dramatically with A due to sampling of spin/isospin sampling.**

GFMC without and with a three-body force

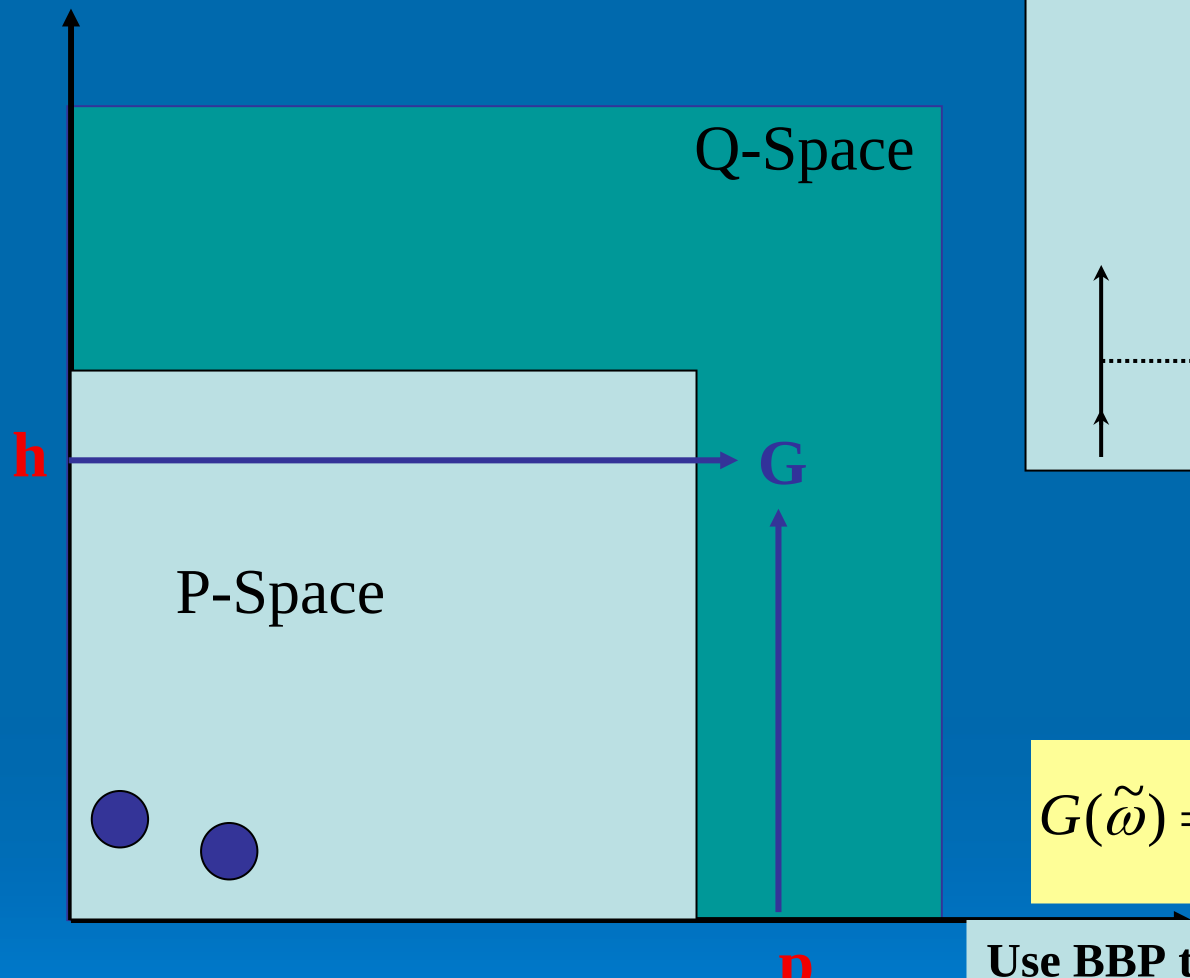


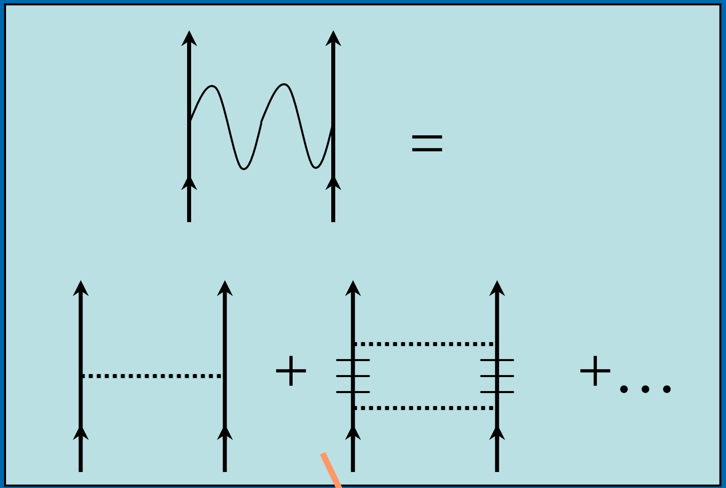
GFMC results for light nuclei



S. C. Pieper and R. B. Wiringa, Ann.Rev.Nucl.Part.Sci. 51 (2001) 53

Choice of model space and the G-matrix





ph intermediate states

$$G(\tilde{\omega}) = V + V\frac{Q}{\tilde{\omega} - QtQ}G(\tilde{\omega})$$

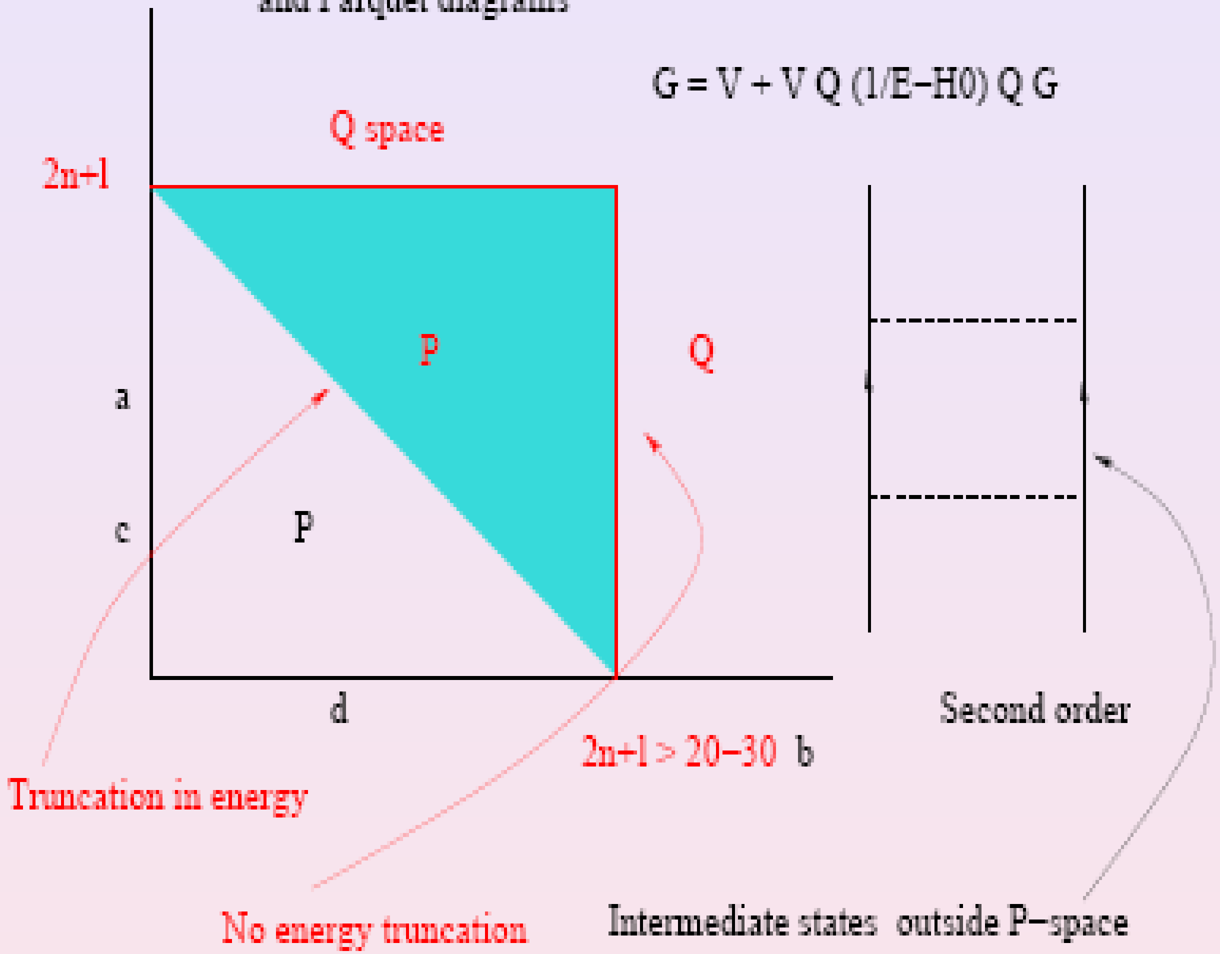
Use BBP to eliminate w-dependence below fermi surface.

$$H = \sum_{pq} \langle p | t_{osc} | q \rangle a_p^+ a_q + \frac{1}{4}\sum_{pqrs} \langle pq | G | rs \rangle a_p^+ a_q^+ a_s a_r$$

Set up a 2-particle 'renormalized' interaction in the model space

Pauli operator for no−core calculations and Coupled cluster and Parquet diagrams

$$G = V + V\,Q\,(1/E-H0)\,Q\,G$$



| ab > is in Q−space and included as intermediate state in G

| cd > is not included in G

Similarity transformed H

$$H\left|k\right\rangle = E_k\left|k\right\rangle; P + Q = 1$$

$$Qe^{-\omega}He^{\omega}P = 0 \quad \Rightarrow \quad \left\langle \alpha_Q \middle| k \right\rangle = \sum_{\alpha_P} \left\langle \alpha_Q \middle| \omega \middle| \alpha_P \right\rangle \left\langle \alpha_P \middle| k \right\rangle$$

$$\overline{H}_{eff} = \left[P\left(1+\omega^{+}\omega\right)P\right]^{1/2} PH\left(P+Q\omega P\right)\left[P\left(1+\omega^{+}\omega\right)P\right]^{-1/2}$$

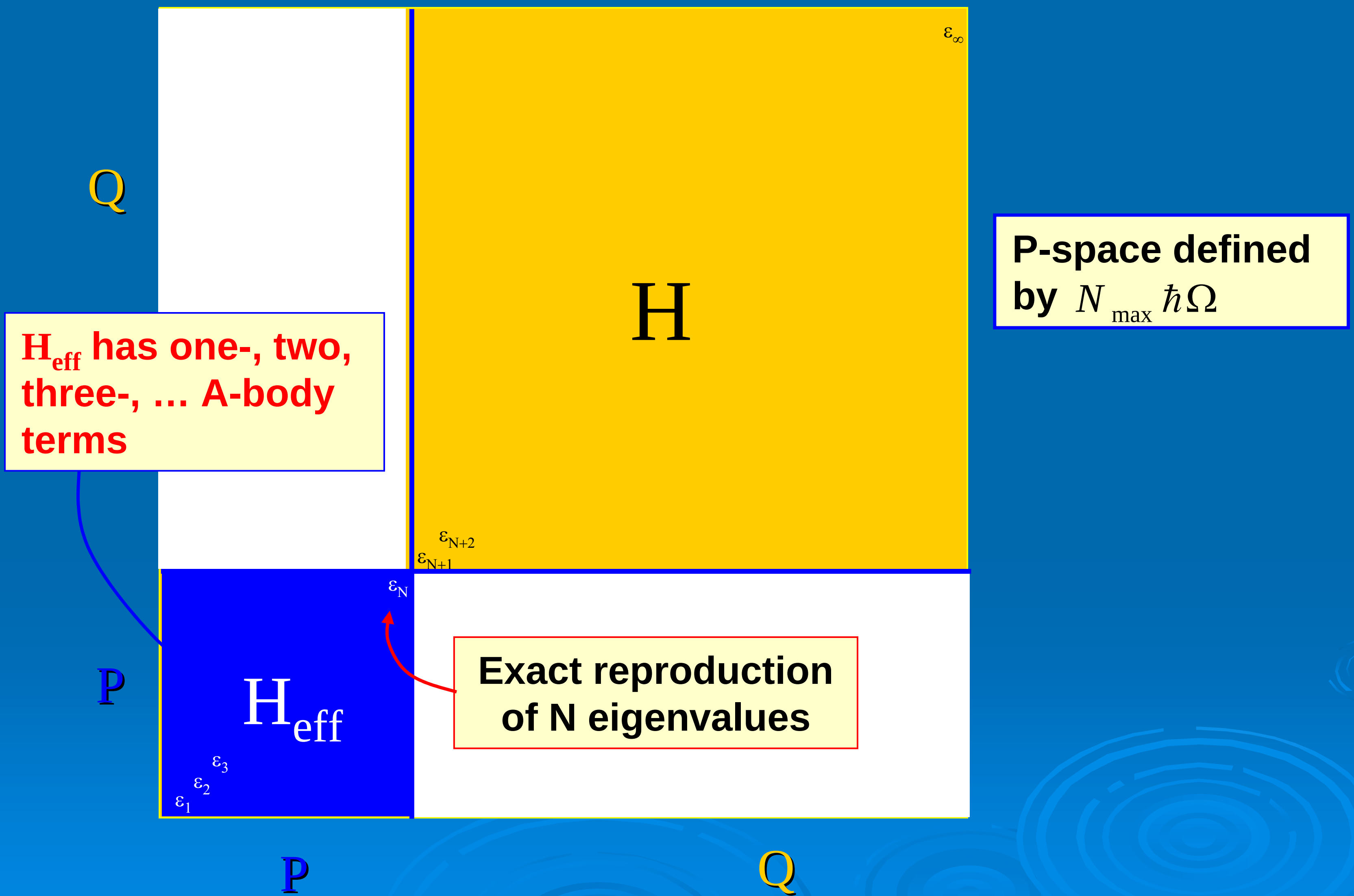
K. Suzuki and S.Y. Lee, Prog. Theor. Phys. 64, 2091 (1980)
P. Navratil, G.P. Kamuntavicius, and B.R. Barrett, Phys. Rev. C61, 044001 (2000)
Zuker, Phys. Repts. (1981); Okubu

Advantage: less parameter dependence in the interaction

Current status

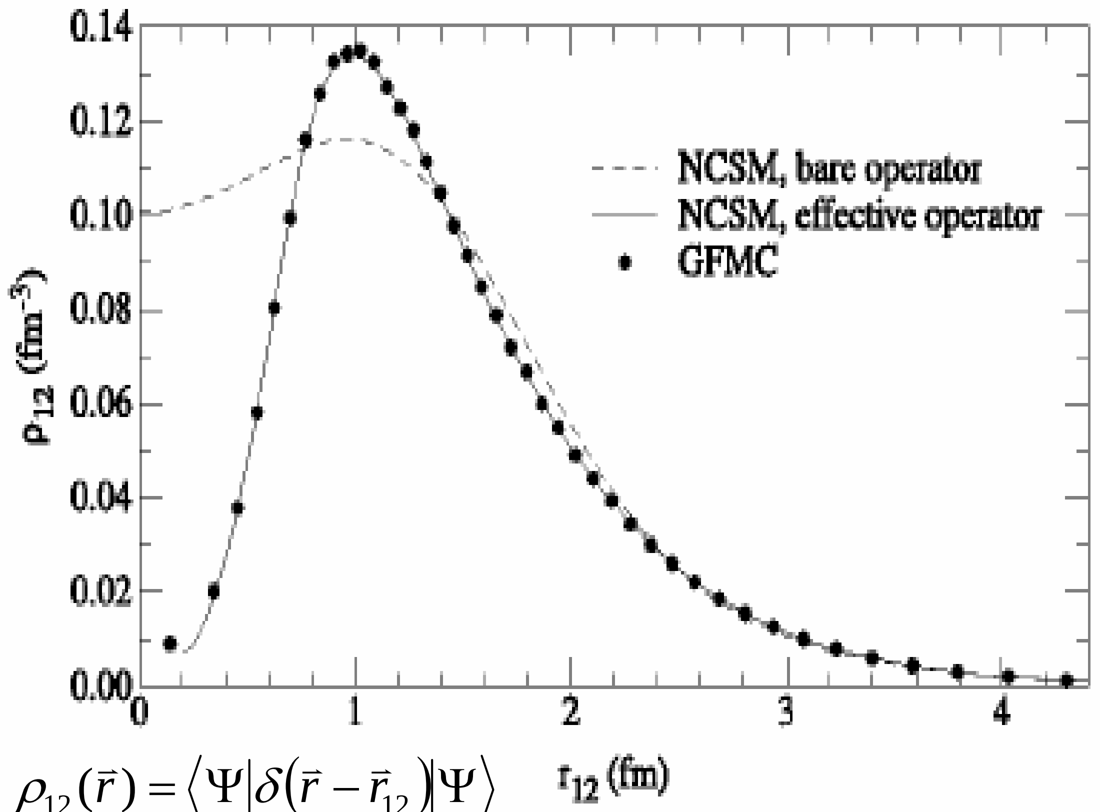
- **Exact deuteron energy obtained in P space**
- **Working on full implementation in CC theory.**
- **G-matrix + all folded-diagrams+…**
- **Implemented, results coming soon….**

The general idea behind Lee-Suzuki



The effective interaction is not the only story. Effective operators can be found within this formalism too...

H. Kamada, *et al.*, Phys. Rev. C 64, 044011 (2001)



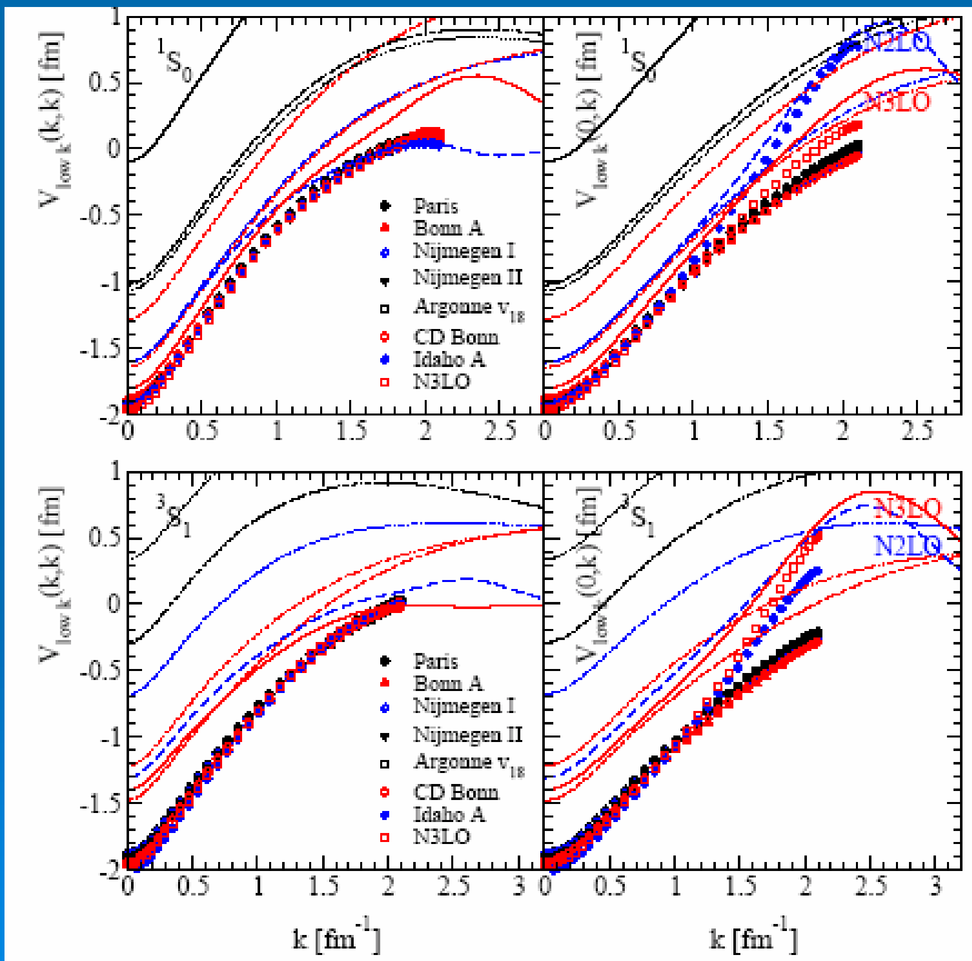
$$\rho_{12}(\vec{r}) = \langle \Psi | \delta(\vec{r} - \vec{r}_{12}) | \Psi \rangle$$

Figure 2. *NCSM and GFMC NN pair density in ^4He.*

Another approach: V_{lowk}

$$T(k',k;k^2) = V_{\rm NN}(k',k) + \frac{2}{\pi}\mathcal{P}\int_0^\infty \frac{V_{\rm NN}(k',p)\,T(p,k;k^2)}{k^2-p^2}\,p^2dp,$$

$$T(k',k;k^2) = V^{\Lambda}_{\rm low\,k}(k',k) + \frac{2}{\pi}\mathcal{P}\int_0^\Lambda \frac{V^{\Lambda}_{\rm low\,k}(k',p)\,T(p,k;k^2)}{k^2-p^2}\,p^2dp.$$



$$\frac{d}{d\Lambda}V^{\Lambda}_{\rm low\,k}(k',k) = \frac{2}{\pi}\frac{V^{\Lambda}_{\rm low\,k}(k',\Lambda)\,T^{\Lambda}(\Lambda,k;\Lambda^2)}{1-(k/\Lambda)^2}$$

Method due to Schwenk, Bogner, Brown, Kuo

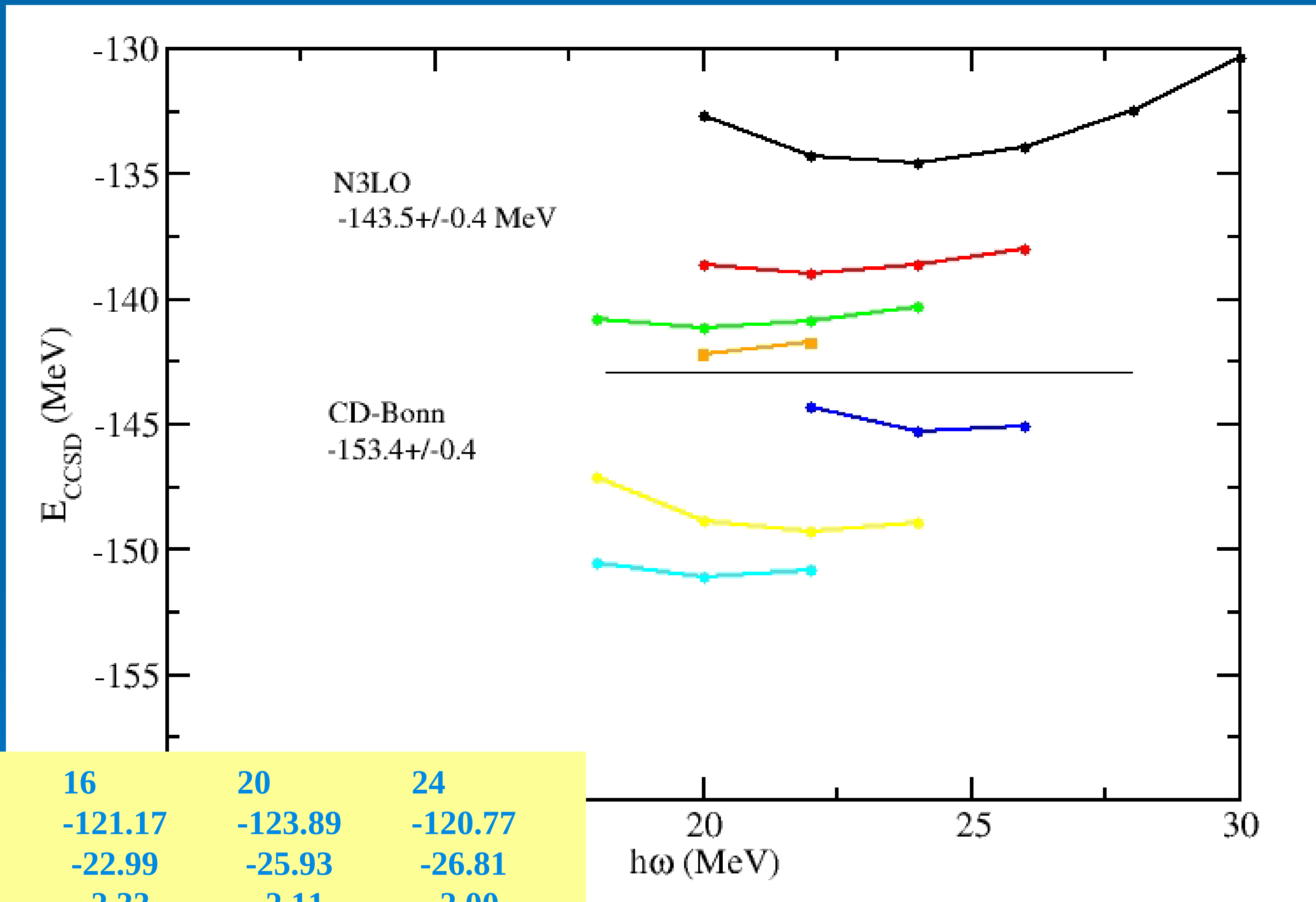
Produces a phase-equivalent potential that may then be used in many-body calculations.

The potentials over bind.

Must be augmented by a 3-body force.

This approach does engender controversy, but it does merit investigations.

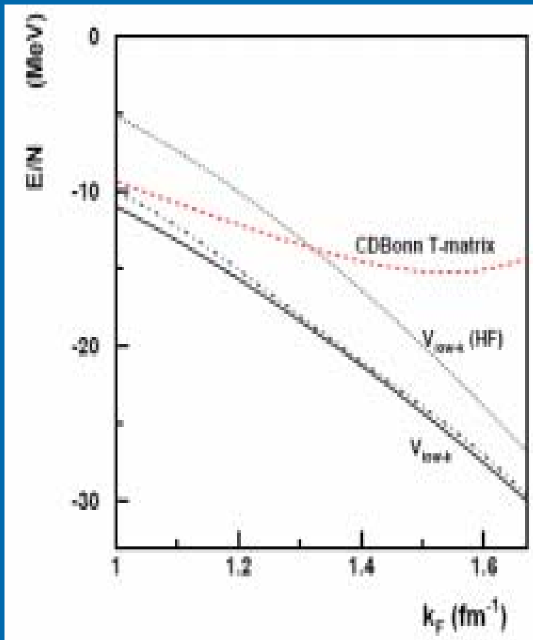
V_{lowk} ^{16}O results using N3LO and CD-Bonn

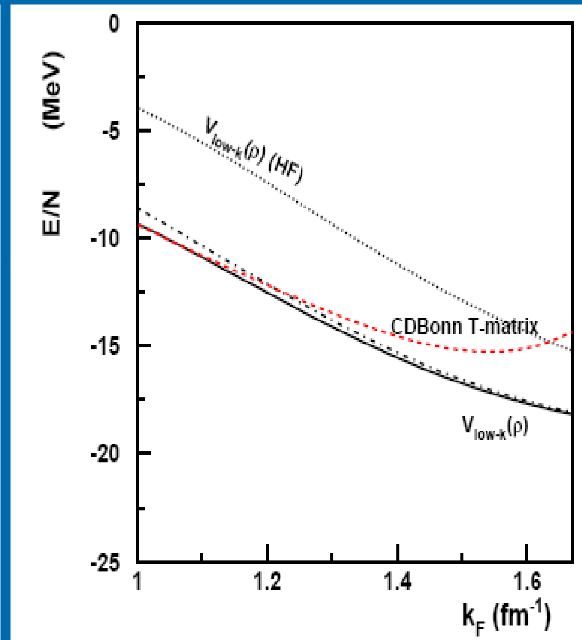


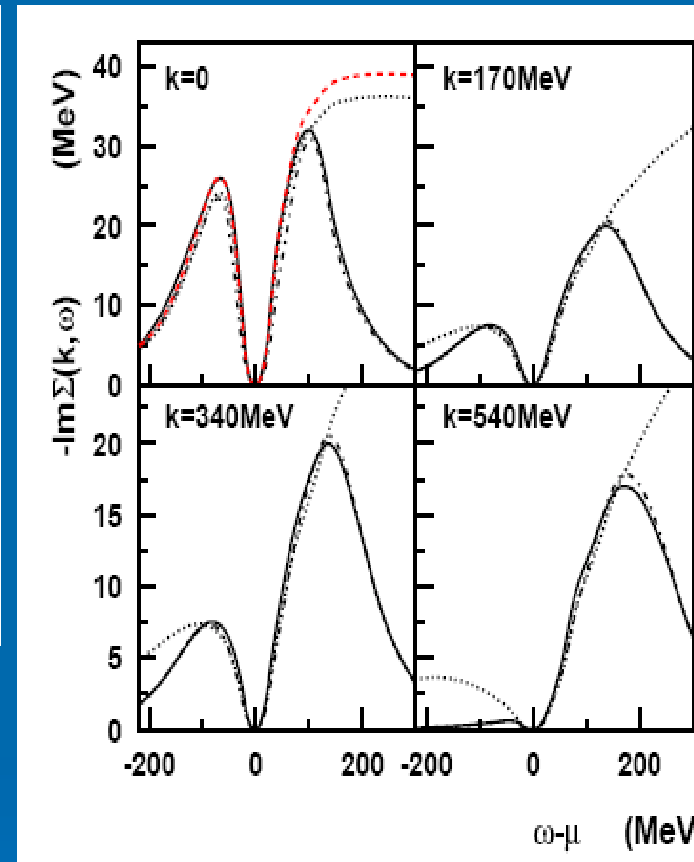
hw	16	20	24
HF	-121.17	-123.89	-120.77
D2	-22.99	-25.93	-26.81
D3	-2.33	-2.11	-2.00
total	-146.49	-151.93	-149.58

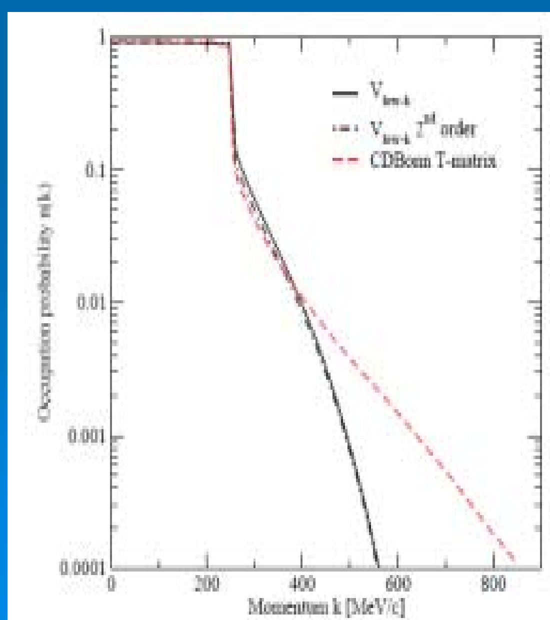
(R. Roth, p.c. – N=6 shells, Λ=2.1 fm^{-1})

Some studies of V_{lowk} in nuclear matter









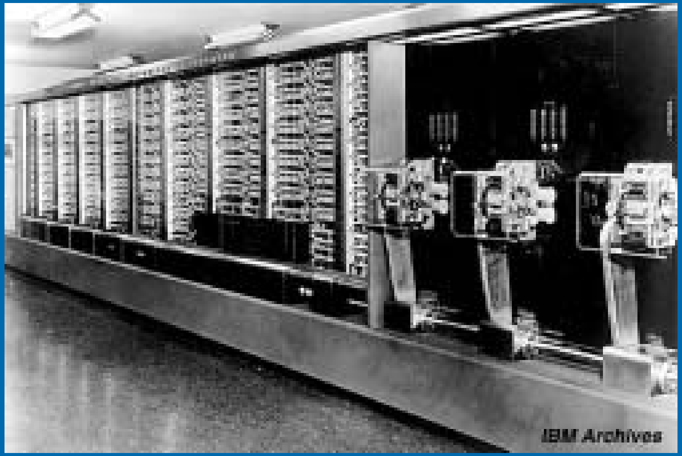
Bozek, Dean, Muether, PRC in press 2006

The ‘advent’ of modern computing and the future

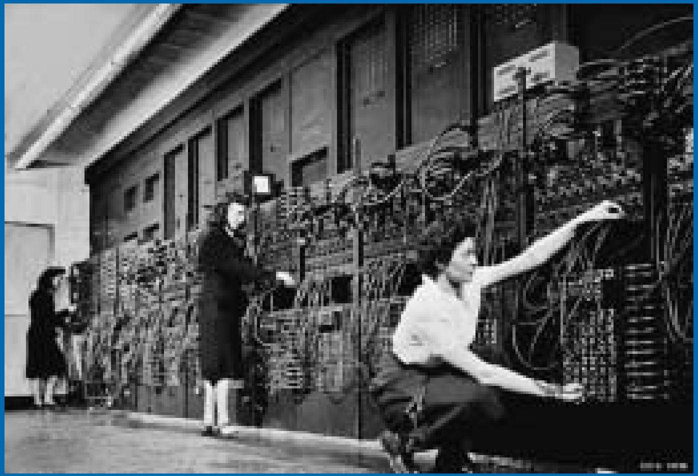
-- 1871: Babbage difference engine
-- Partially built as Babbage ran out of funds.
-- Working model built in 1991; 31 digit numerical accuracy.

Moore’s law has affected the leading edge of computing for decades….

Supercomputing of the 1940's



1943, Harvard Mark-I



1946, ENIAC

1946, Metropolis Monte Carlo (von Neumann)

1947, Wirlwind, MIT

1947, invention of transistors and magnetic drum memory

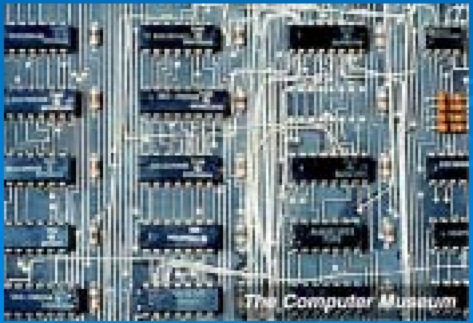
Supercomputing of the 1950's

1953, ORACLE
Oak Ridge Automated
Computer and Logic Engine

1957, GEORGE at Argonne
16 k, memory, paper tape I/O

1954, FORTRAN developed by John Backus

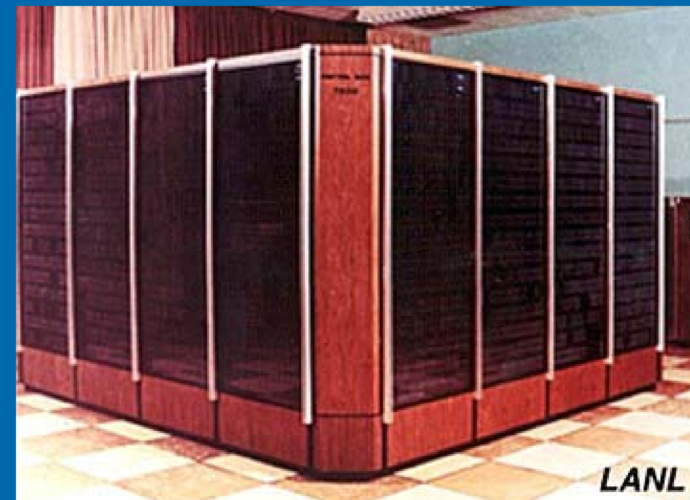
1959, Robert Noyce and Gordan Moore file patent for integrated curcuit



1957, Lax method yields stable
fluid flow and hydrodynamics algorithms

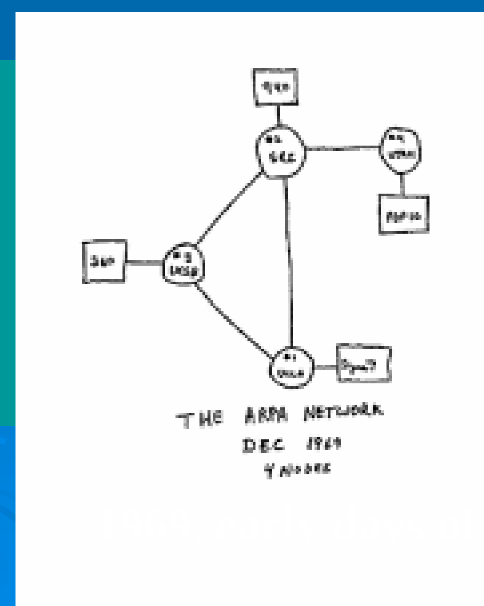
Supercomputing of the 1960s

1964, CDC6600, first commercially successful supercomputer; 9 MFlops



1969, CDC760, 40 Mflops

1965: The ion-channeling effect, one of the first materials physics discoveries made using computers, is key to the ion implantation used by current chip manufacturers to "draw" transistors with boron atoms inside blocks of silicon.



the internet.

1967, Computer simulations used to calculate radiation dosages.

Supercomputing of the 1970s and 1980s

1974, IBM 370/195 to Argonne

1983, Carbon Dioxide Information Analysis Center (Climate modeling)

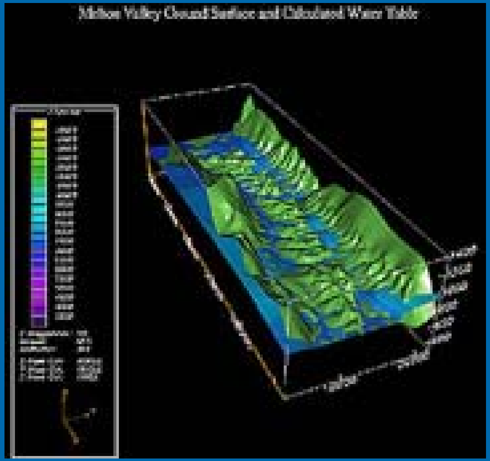
1974, Controlled Thermonuclear Research Computer Center (precursor to NERSC) established

1979, Breakthroughs in neural networks

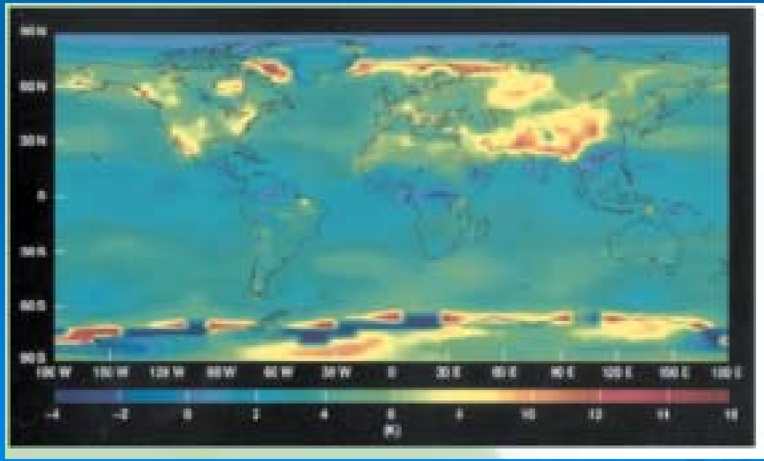
1983, CRAY-XMP

Supercomputing of the 1980s

1983, first 8-processor CRAY-II delivered to NERSC



1988, 3D FEMWATER
Water flow through porous media

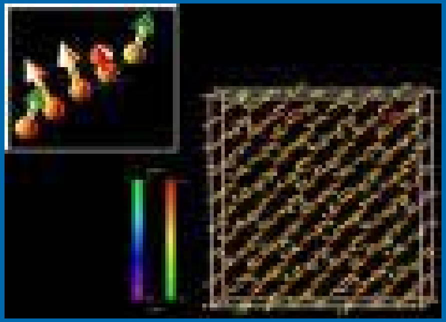


Early Climate Modeling

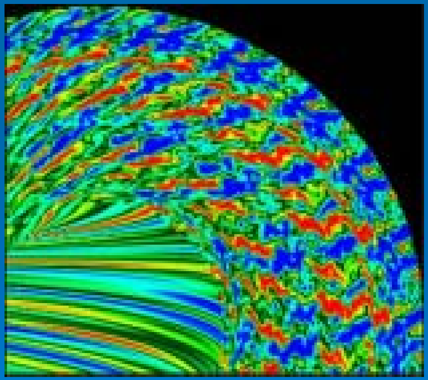
1985, Thinking Machines, Connection Machine, 1 Gflop

Supercomputing of the 1990s

1993, CRAY-T3D, NERSC



1998, spin system, Gordon Bell Prize
1 Tflop on T3E.



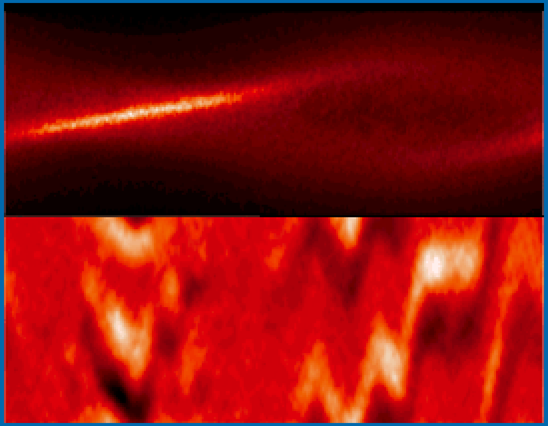
1991, TORT, 3D deterministic radiation transport code

1994, Netscape invented at NCSA

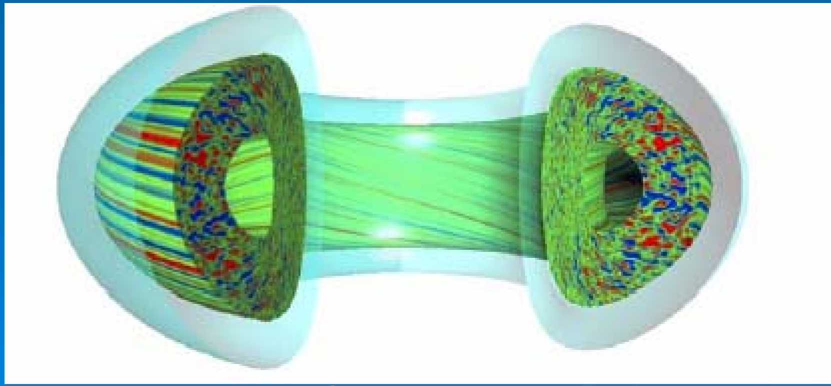
2000, ORNL Eagle (IBM SP)

Office of Science Computing Today

NERSC: IBM/RS6000
(9.1 TFlops peak)



2001, Dispersive waves in magnetic reconnection

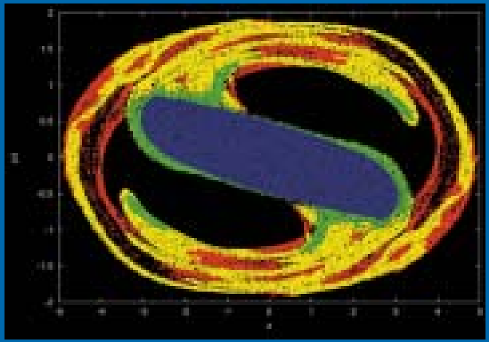


2003, Turbulent flow in Tokomak Plasmas

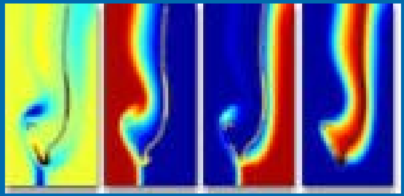
CRAY-X1 at ORNL

Today's science on today's computers

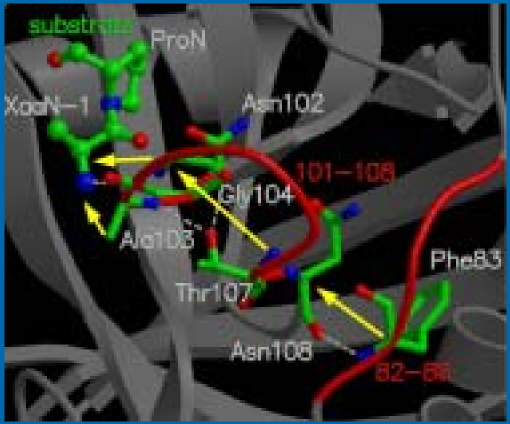
Type IA supernova explosion (BIG SPLASH)



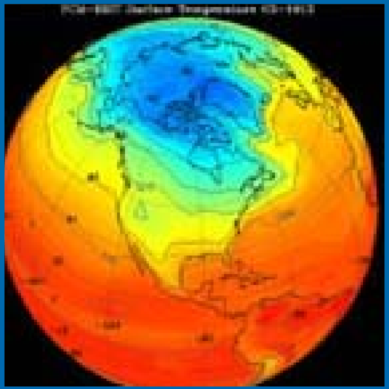
Accelerator design



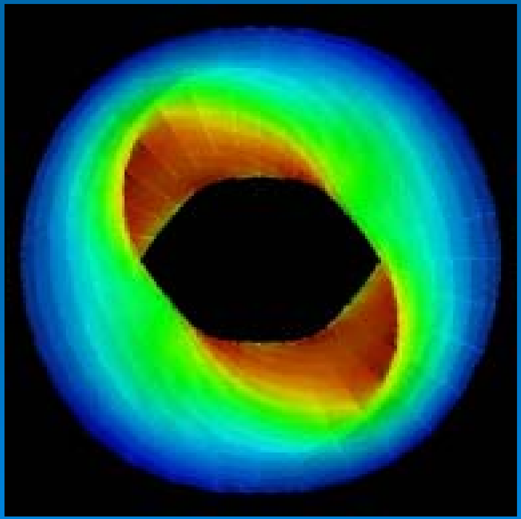
Reacting flow science



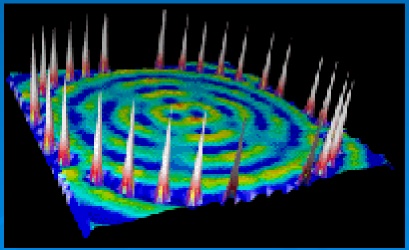
Multiscale model of HIV



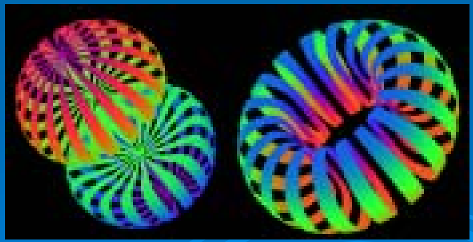
Atmospheric models



Fusion Stellarator

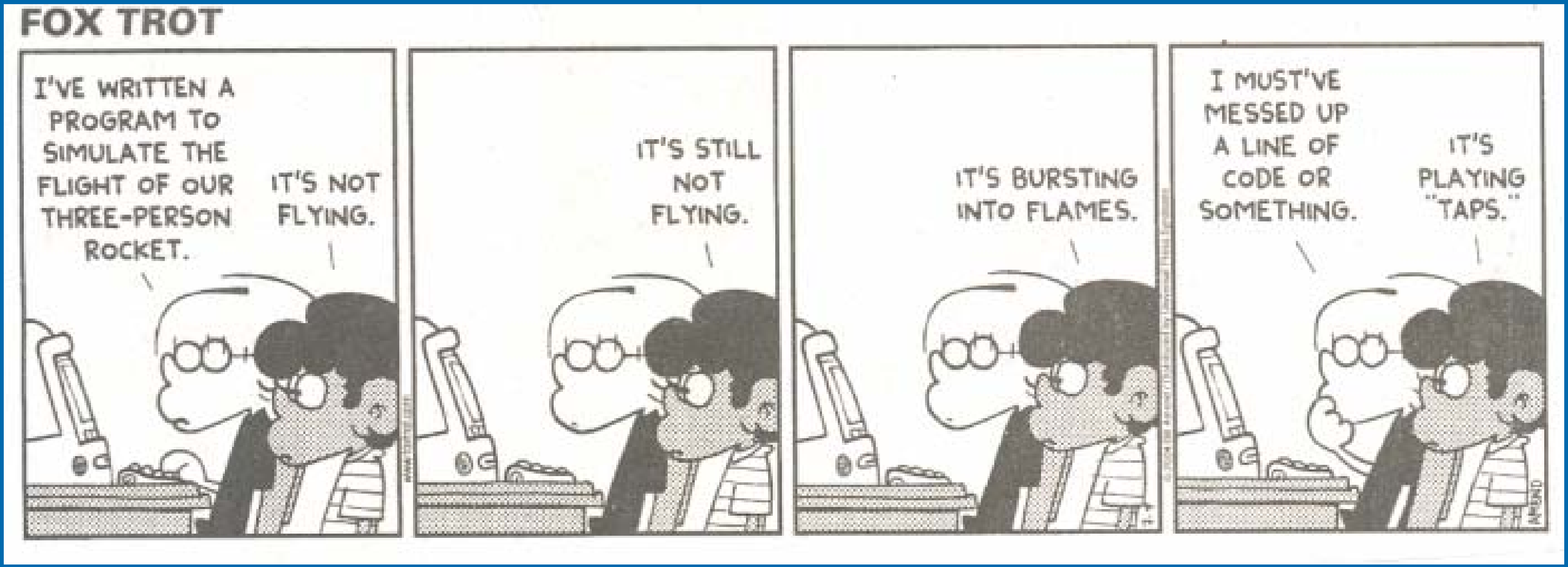


Materials: Quantum Corral



Structure of deutrons and nuclei

"I always thought that record would stand until it was broken" YB



Verification and Validation (V&V)

Doing the problem right. – Verify
Doing the right problem. – Validate

Building a coherent theoretical path forward

Inter-nucleon
NN, NNN interactions
EFT, AV18,…

Many-body theory
Spectroscopy and selected reactions
Method verification
Experimental validation
Expansion to mass 100

Density Functional Theory
Improved functionals
Remove imposed constraints
Wave functions for nuclei A>16

DFT Dynamical extensions
LACM and spectroscopy by projection, GCM, TDDFT, QRPA

Improved low-energy reactions
Hauser-Feshbach
Pre-equilibrium emission
fission mass and energy distributions
Optical potentials; level densities

Main point today:

- Moving from NN and NNN to many-body calculations

The nuclear Hamiltonian

$$H = -\frac{\hbar}{2}\sum_{i=1}^{A}\frac{\nabla_i^2}{m_i} + \frac{1}{2}\sum_{i<j} V_{2N}\left(\vec{r}_i, \vec{r}_j\right) + \frac{1}{6}\sum_{i<j<k} V_{3N}\left(\vec{r}_i, \vec{r}_j, \vec{r}_k\right)$$

$$\left\langle pq \| rs \right\rangle = \left\langle pq \middle| V(\vec{r}_1, \vec{r}_2) \middle| rs \right\rangle = \int d\vec{r}_1 d\vec{r}_2 \phi_p^*(\vec{r}_1)\phi_q^*(\vec{r}_2) V(\vec{r}_1, \vec{r}_2)\phi_r(\vec{r}_1)\phi_s(\vec{r}_2)$$

⬇

$$H = \sum_{pq}\left\langle p \middle| t \middle| q \right\rangle a_p^+ a_q + \frac{1}{4}\sum_{pqrs}\left\langle pq \middle| V \middle| rs \right\rangle a_p^+ a_q^+ a_s a_r$$

⬇

$$H = \sum_{pq}\left\langle p \middle| t \middle| q \right\rangle a_p^+ a_q + \frac{1}{4}\sum_{pqrs}\left\langle pq \middle| V_{\text{eff}} \middle| rs \right\rangle a_p^+ a_q^+ a_s a_r$$

Any questions to this point? Any concerns?

The harmonic oscillator basis is not translationally invariant!

$$H = T - T_{CM} + V + \beta_{CM} H_{CM}$$

“Lawson” term

General many-body problem for fermions (basis expansions)

→ particles are spin ½ fermions
→ many-body wave function is fully anti-symmetric
→ certain quantum numbers will be conserved

for nuclei: total angular momentum
total parity
'isospin' (analogous to spin)
'isospin projection, $T_z = (N-Z)/2$

→ Hamiltonian will be non-relativistic (usually)
→ We (usually) work in second quantization

Fock space with N single particle states and A particles.

$$a_\alpha^+|0\rangle = |1\rangle \quad a_\alpha|0\rangle = 0 \quad a_\alpha|1\rangle = |0\rangle \quad a_\alpha^+|1\rangle = 0$$

$$a_\alpha^+ a_\beta^+ = -a_\beta^+ a_\alpha^+ \quad a_\alpha a_\beta = -a_\beta a_\alpha \quad a_\alpha^+ a_\beta + a_\beta a_\alpha^+ = \delta_{\alpha\beta}$$

$$|\Phi\rangle = a_1^+ a_2^+ \cdots a_A^+|0\rangle = |11\cdots10000\rangle$$

Lowest order many-body theory: Hartree-Fock

$$H|\Psi\rangle = E|\Psi\rangle \quad E[\Psi] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \quad \delta E[\Psi] = 0 \quad \langle\delta\Psi|H - E|\Psi\rangle = 0$$

For a coordinate space calculation

$$E_1 = \langle\Psi|H_1|\Psi\rangle = \sum_\alpha \int d\vec{r}\, \psi_\alpha^*(\vec{r}) \frac{-\hbar^2\nabla^2}{2m} \psi_\alpha(\vec{r})$$

$$\delta E_1 = \frac{\delta}{\delta\psi_\kappa^*(\vec{r}\,')} \sum_\alpha \int d\vec{r}\, \psi_\alpha^*(\vec{r}) \frac{-\hbar^2\nabla^2}{2m} \psi_\alpha(\vec{r}) = \sum_\alpha \int d\vec{r}\, \delta_{\kappa\alpha} \delta(\vec{r}\,' - \vec{r}) \frac{-\hbar^2\nabla^2}{2m} \psi_\alpha(\vec{r})$$

$$= \frac{-\hbar^2\nabla^2}{2m} \psi_\kappa(\vec{r}\,')$$

$$E_2 = \langle\Psi|H_2|\Psi\rangle = \sum_{\alpha\beta} \int d\vec{r}_1 d\vec{r}_2 \left(\psi_\alpha^*(\vec{r}_1)\psi_\beta^*(\vec{r}_2) - \psi_\beta^*(\vec{r}_1)\psi_\alpha^*(\vec{r}_2)\right) V(\vec{r}_1, \vec{r}_2) \psi_\alpha(\vec{r}_1)\psi_\beta(\vec{r}_2)$$

$$\delta E_2 = \frac{\delta}{\delta\psi_\kappa^*(\vec{r}\,')} E_2 = \sum_{\alpha\beta} \int d\vec{r}_1 d\vec{r}_2 \left(\delta_{\alpha\kappa}\delta(\vec{r}_1 - \vec{r}\,')\psi_\beta^*(\vec{r}_2) - \delta_{\beta\kappa}\delta(\vec{r}_1 - \vec{r}\,')\psi_\alpha^*(\vec{r}_2)\right) V(\vec{r}_1, \vec{r}_2) \psi_\alpha(\vec{r}_1)\psi_\beta(\vec{r}_2)$$

$$= \sum_{\alpha\beta} \int d\vec{r}_2 \left(\delta_{\alpha\kappa}\psi_\beta^*(\vec{r}_2) - \delta_{\beta\kappa}\psi_\alpha^*(\vec{r}_2)\right) V(\vec{r}\,', \vec{r}_2) \psi_\alpha(\vec{r}\,')\psi_\beta(\vec{r}_2)$$

$$= \sum_\beta \int d\vec{r}_2 \psi_\beta^*(\vec{r}_2) V(\vec{r}\,', \vec{r}_2) \psi_\kappa(\vec{r}\,')\psi_\beta(\vec{r}_2) - \sum_\alpha \int d\vec{r}_2 \psi_\alpha^*(\vec{r}_2) V(\vec{r}\,', \vec{r}_2) \psi_\alpha(\vec{r}\,')\psi_\kappa(\vec{r}_2)$$

Hartree-Fock II

Putting it all together

$$\delta E = \frac{-\hbar^2\nabla^2}{2m}\psi_\kappa(\vec{r}\,') + \sum_\beta \int d\vec{r}_2 \psi_\beta^*(\vec{r}_2) V(\vec{r}\,',\vec{r}_2)\psi_\kappa(\vec{r}\,')\psi_\beta(\vec{r}_2) - \sum_\alpha \int d\vec{r}_2 \psi_\alpha^*(\vec{r}_2) V(\vec{r}\,',\vec{r}_2)\psi_\alpha(\vec{r}\,')\psi_\kappa(\vec{r}_2)$$

$$\rho(\vec{r}) = \sum_\alpha \psi_\alpha^*(\vec{r})\psi_\alpha(\vec{r}) \qquad \rho(\vec{r},\vec{r}\,') = \sum_\alpha \psi_\alpha^*(\vec{r})\psi_\alpha(\vec{r}\,')$$

$$\frac{-\hbar^2\nabla^2}{2m}\psi_\kappa(\vec{r}\,') + \int d\vec{r}_2 \rho(\vec{r}_2) V(\vec{r}\,',\vec{r}_2)\psi_\kappa(\vec{r}\,') - \int d\vec{r}_2 \rho(\vec{r}_2,\vec{r}\,') V(\vec{r}\,',\vec{r}_2)\psi_\kappa(\vec{r}_2) = e_\kappa \psi_\kappa(\vec{r})$$

Direct term (easy)

Exchange term (hard)

$$\left[\frac{-\hbar^2\nabla^2}{2m} + \Gamma_H(\vec{r}\,')\right]\psi_\kappa(\vec{r}\,') - \int d\vec{r}_2 \Gamma_{Ex}(\vec{r}\,',\vec{r}_2)\psi_\kappa(\vec{r}_2) = e_\kappa \psi_\kappa(\vec{r})$$

Hartree Fock in a basis

Definition of HF: one single slater determinant describes the ground state of the system. "Interaction of one particle with the average potential describing the rest of the system."

$$H = \sum_{pq} \langle p|t|q\rangle a_p^+ a_q + \frac{1}{4}\sum_{pqrs}\langle pq|V|rs\rangle a_p^+ a_q^+ a_s a_r$$

$$\psi_i^{\mathrm{HF}} = \sum_k D_{ki}\varphi_k \qquad c_i^+ = \sum_k D_{ki} a_k^+$$

$$E_{HF} = \langle \Psi_{HF}|H|\Psi_{HF}\rangle = E_{HF}[\rho] = \sum_{pq} t_{pq}\langle \Psi_{HF}|a_p^+ a_q|\Psi_{HF}\rangle + \frac{1}{4}\sum_{pqrs}\bar{V}_{pqrs}\langle \Psi_{HF}|a_p^+ a_q^+ a_s a_r|\Psi_{HF}\rangle$$

$$= \sum_{pq} t_{pq}\rho_{qp} + \frac{1}{2}\sum_{pqrs}\rho_{rp}\bar{V}_{pqrs}\rho_{sq}$$

$$E_{HF} = \sum_{i=1}^{A} t_{ii} + \frac{1}{2}\sum_{i,j=1}^{A}\bar{V}_{ijij}$$

Hartree-Fock in a basis

$$\frac{\partial E^{HF}[\rho]}{\partial \rho_{kk'}} \delta\rho_{kk'} = \sum_{kk'} \left[t_{kk'} + \sum_{ll'} \bar{V}_{kl'k'l} \rho_{ll'} \right] \delta\rho_{kk'}$$

yields a set of coupled, non-linear differential equations;
in a basis yields an eigenvalue problem:

$$\sum_i \left(t_{ij} + \sum_{ll'} \bar{v}_{iljl'} \rho_{l'l} \right) D_{jk} = \varepsilon_k D_{ik}$$

$$\rho_{ll'} = \sum_{i=1}^{A} D_{li}^* D_{l'i}$$

one-body term

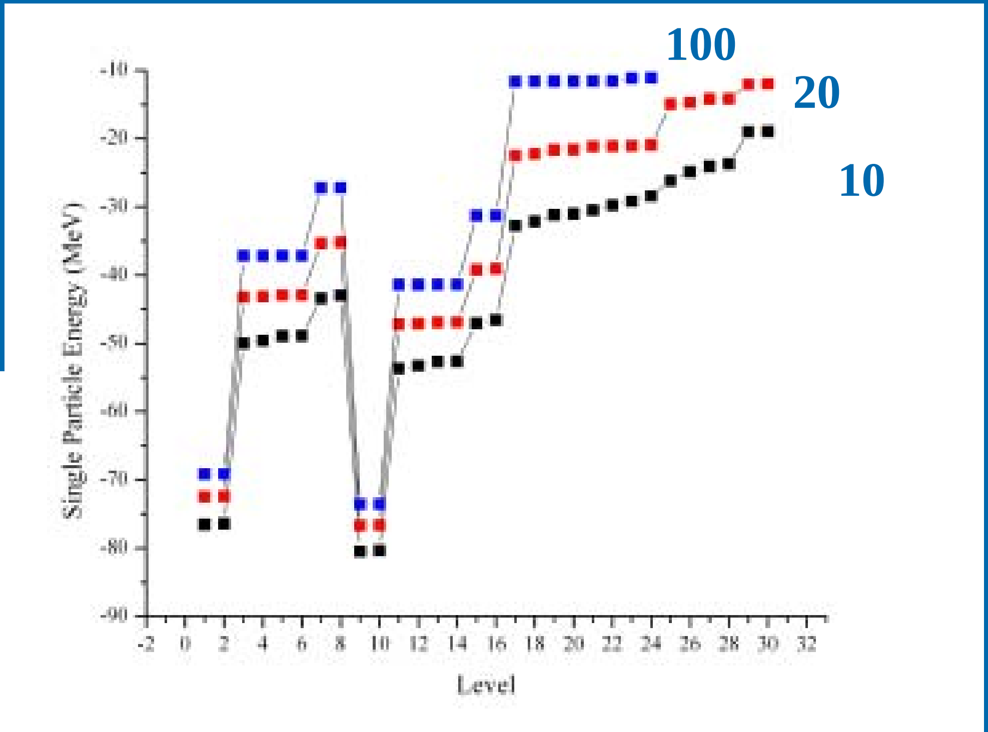
$$\bar{V}_{ijkl} = \langle \varphi_i \varphi_j | V | \varphi_k \varphi_l \rangle - \langle \varphi_i \varphi_j | V | \varphi_l \varphi_k \rangle$$

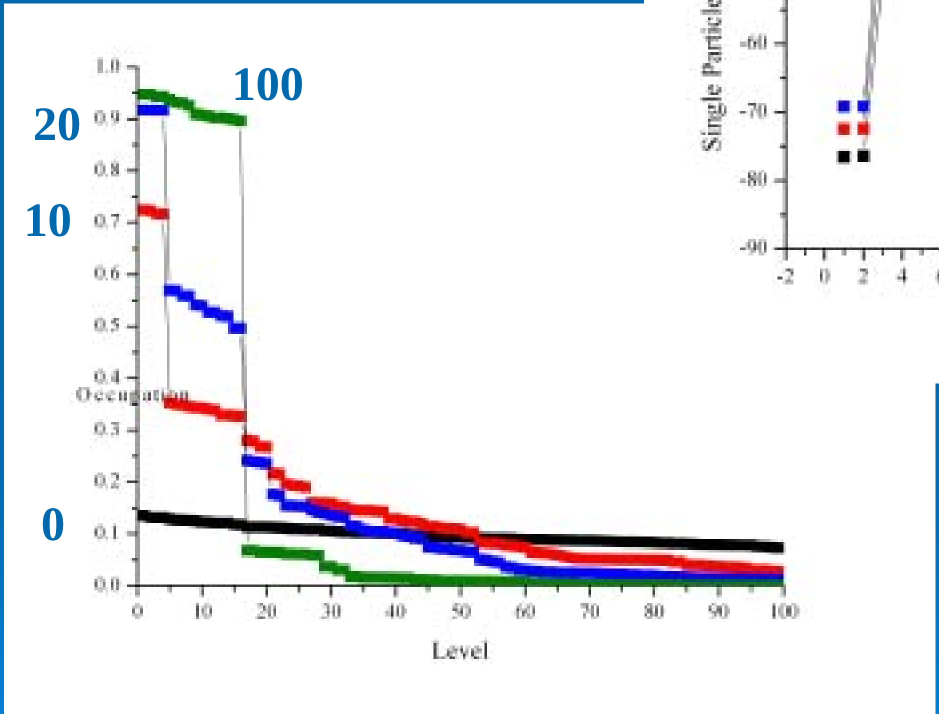
$$\varphi_i^{\mathrm{HF}} = \sum_k D_{ki} \psi_k$$

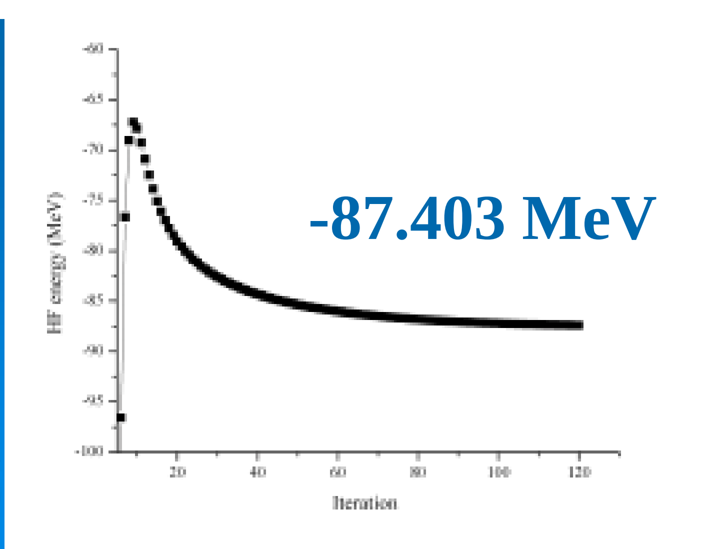
HF calculations yield:
- Single-particle energies
- HF basis interaction matrix elements

Hartree-Fock iterative solutions

$$H = T - T_{CM} + V$$

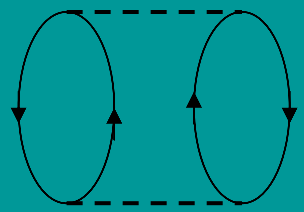






Many-body perturbation theory

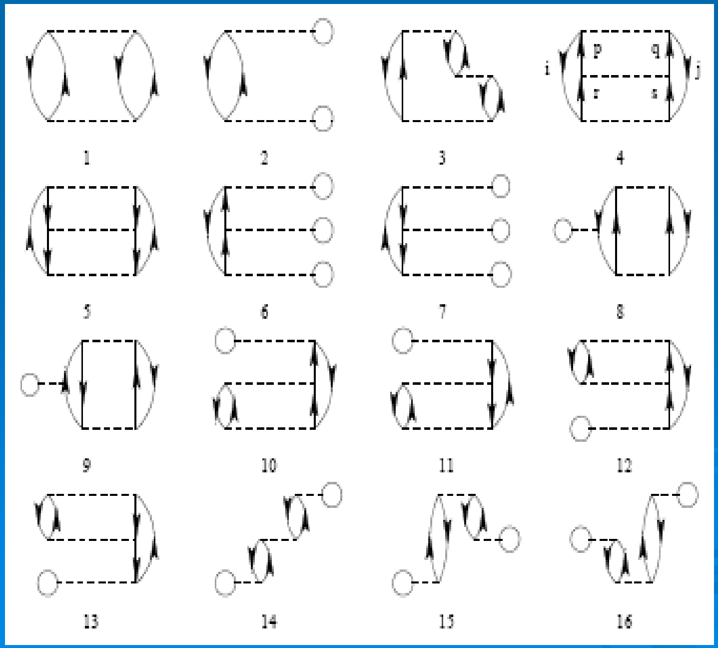
2nd order



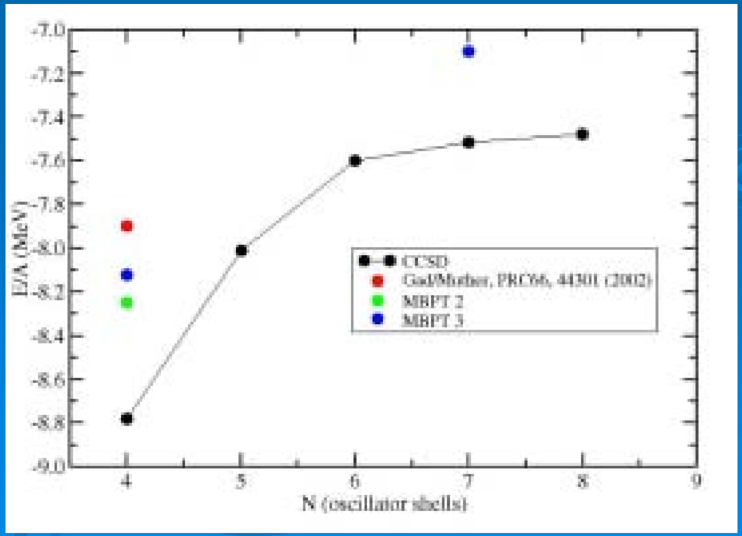
$$E_2 = \sum_{\substack{a>b \\ i>j}} \frac{\langle ab \| ij \rangle \langle ab \| ij \rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

-36.1325 MeV

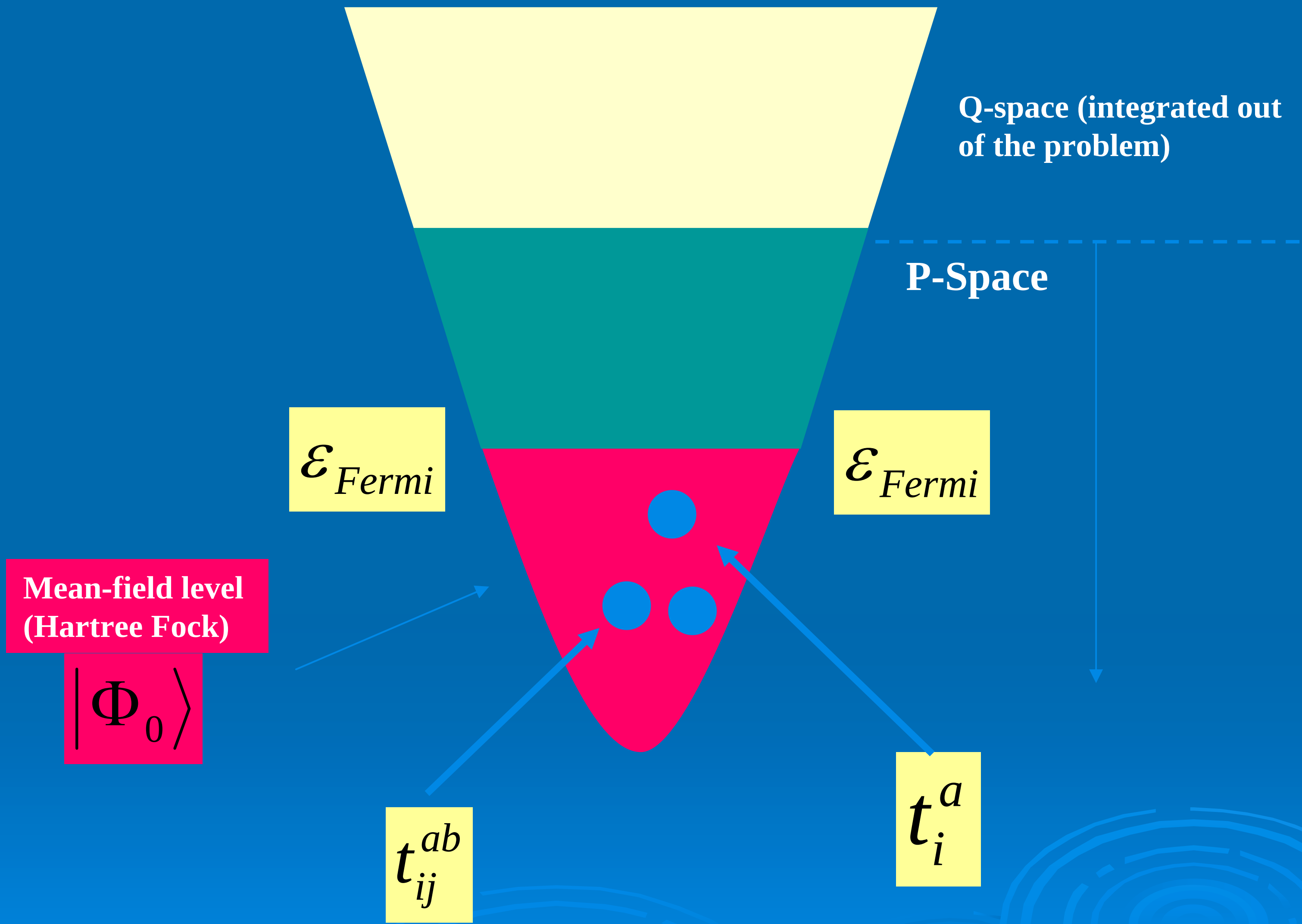
$E=E_{HF}+E_2=-123.55$ MeV



comparison of CC and MBPT

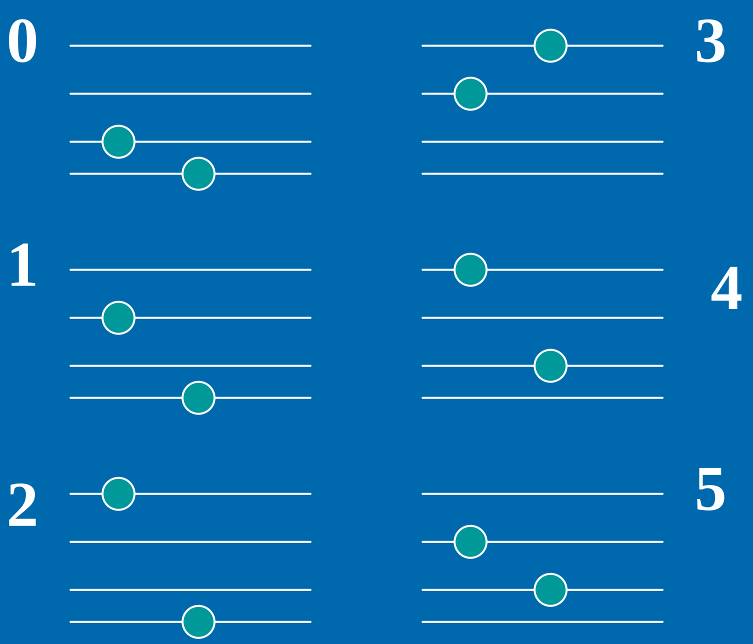


Interactions within the P-space



$$H = \sum_{pq} \langle p | t_{osc} | q \rangle a_p^+ a_q + \frac{1}{4} \sum_{pqrs} \langle pq | G | rs \rangle a_p^+ a_q^+ a_s a_r$$

Specific example: 2 particles in 4 states



$$I=0 \quad a_2^+ a_1^+ \left|--\right\rangle = \left|1100\right\rangle = \left|\Phi_0\right\rangle$$

$$I=1 \quad a_3^+ a_1^+ \left|--\right\rangle = \left|1010\right\rangle = \left|\Phi_1\right\rangle$$

$$I=2 \quad a_4^+ a_1^+ \left|--\right\rangle = \left|1001\right\rangle = \left|\Phi_2\right\rangle$$

$$I=3 \quad a_3^+ a_2^+ \left|--\right\rangle = \left|0110\right\rangle = \left|\Phi_3\right\rangle$$

$$I=4 \quad a_4^+ a_2^+ \left|--\right\rangle = \left|0101\right\rangle = \left|\Phi_4\right\rangle$$

$$I=5 \quad a_4^+ a_3^+ \left|--\right\rangle = \left|0011\right\rangle = \left|\Phi_5\right\rangle$$

Scaling: Number of basis states

Oops. These are HUGE numbers

$n =$ number of particles;

$N =$ number of single-particle states

$$C(N,n) = \frac{N!}{(N-n)!\,n!}$$

$$C(10,100) = 1.7x10^{13}$$

$$C(1000,100) = 6x10^{139}$$

PROBLEM : How to deal with such large dimensions???

Correlated wave function representation

We have a complete set of states that span our truncated Hilbert space:

$$1 = \sum_{I=0}^{N-1} |I\rangle\langle I|; \quad \langle I | J \rangle = \delta_{IJ}$$

"mean field" → Uncorrelated state of lowest energy.

$$|\Phi_0\rangle = |1100\rangle$$

$$|\Psi_\alpha\rangle = \left(b_\alpha + b_\alpha^{ai} a_a^+ a_i + b_\alpha^{abij} a_a^+ a_b^+ a_i a_j + \cdots\right)|\Phi_0\rangle$$

1p-1h 2p-2h … np-nh

(implicit summation assumed)

$$1 = \sum_{\alpha=0}^{N-1} |\Psi_\alpha\rangle\langle\Psi_\alpha|; \langle\Psi_\alpha|\Psi_\beta\rangle = \delta_{\alpha\beta}$$

Problem II: How do we solve for the correlated many-body wave function?

Diagonal contributions to the Hamiltonian matrix

Here we apply Wick's theorem to the one-body term and the diagonal contributions of the two-body term.

$$H_{11} \leftarrow \varepsilon_1 \langle --| a_1 a_2 a_1^+ a_1 a_2^+ a_1^+ |--\rangle + \varepsilon_2 \langle --| a_1 a_2 a_2^+ a_2 a_2^+ a_1^+ |--\rangle$$

$$H_{11} \leftarrow \frac{1}{4} V_{1212} \langle --| a_1 a_2 a_1^+ a_2^+ a_2 a_1 a_2^+ a_1^+ |--\rangle = \frac{1}{4} V_{1212}$$

$$\begin{pmatrix} \varepsilon_1 + \varepsilon_2 + \frac{1}{4} V_{1212} & & & & & \\ & \varepsilon_1 + \varepsilon_3 & & & & \\ & & \varepsilon_1 + \varepsilon_4 & & & \\ & & & \varepsilon_3 + \varepsilon_2 & & \\ & & & & \varepsilon_3 + \varepsilon_2 & \\ & & & & & \varepsilon_3 + \varepsilon_4 \end{pmatrix}$$

Two-body contributions to the Hamiltonian matrix

$$V_{1234} = -V_{2134} = -V_{1243} = V_{2143} = V_{3421} = -V_{4321} = -V_{3412} = V_{4312}$$

$$H_{16} \leftarrow \frac{1}{4} V_{1234} \langle --| a_1 a_2 a_1^+ a_2^+ a_4 a_3 a_4^+ a_3^+ |--\rangle = \frac{1}{4} V_{1234}$$

$$H_{61} \leftarrow \frac{1}{4} V_{1234} \langle --| a_3 a_4 a_1^+ a_2^+ a_4 a_3 a_2^+ a_1^+ |--\rangle = 0$$

$$H_{61} \leftarrow \frac{1}{4} V_{3412} \langle --| a_3 a_4 a_3^+ a_4^+ a_2 a_1 a_2^+ a_1^+ |--\rangle = \frac{1}{4} V_{3412}$$

$$H_{43} \leftarrow \frac{1}{4} V_{2314} \langle --| a_2 a_3 a_2^+ a_3^+ a_4 a_1 a_4^+ a_1^+ |--\rangle = \frac{1}{4} V_{2314}$$

$$H_{34} \leftarrow \frac{1}{4} V_{1423} \langle --| a_1 a_4 a_1^+ a_4^+ a_3 a_2 a_3^+ a_2^+ |--\rangle = \frac{1}{4} V_{1423}$$

$$H_{12} \leftarrow \frac{1}{4} V_{1213} \langle --| a_1 a_2 a_1^+ a_4^+ a_3 a_1 a_3^+ a_1^+ |--\rangle = \frac{1}{4} V_{1213}$$

Hamiltonian matrix now 'mixes' bare eigenstates

$$H = \begin{pmatrix}
\varepsilon_1 + \varepsilon_2 + \frac{1}{2}V_{1212} & \frac{1}{4}V_{1213} & & & & \frac{1}{4}V_{1234} \\
\frac{1}{4}V_{1312} & \varepsilon_1 + \varepsilon_3 + \frac{1}{2}V_{1313} & & & & \\
& & \varepsilon_1 + \varepsilon_4 + \frac{1}{2}V_{1414} & \frac{1}{4}V_{2134} & & \\
& & \frac{1}{4}V_{2314} & \varepsilon_2 + \varepsilon_3 + \frac{1}{2}V_{2323} & & \\
& & & & \varepsilon_3 + \varepsilon_4 + \frac{1}{2}V_{3434} & \\
\frac{1}{4}V_{3412} & & & & & \varepsilon_3 + \varepsilon_4 + \frac{1}{2}V_{3434}
\end{pmatrix}$$

Solve the eigen problem

- **Generate the Hamiltonian matrix and diagonalize (Lanczos)**
- **Yields eigenvalues and eigenvectors of the problem**

$$U^{+}_{\alpha J}\langle J|H|I\rangle U_{I\alpha} = \lambda_{\alpha}\langle\alpha|H|\alpha\rangle$$

$$|\alpha\rangle = \sum_{I} U_{I\alpha}|I\rangle$$

$$|\Psi_{\alpha}\rangle = \left(b_{\alpha} + b_{\alpha}^{ai} a_{a}^{+} a_{i} + b_{\alpha}^{abij} a_{a}^{+} a_{b}^{+} a_{i} a_{j} + \cdots\right)|\Phi_{0}\rangle$$

i, j run below the Fermi surface

a, b run above the Fermi surface

Solving the ab-initio quantum many-body problem

Exact or virtually exact solutions available for:

- A=3: solution of Faddeev equation.
- A=4: solvable via Faddeev-Yakubowski approach.
- Light nuclei (up to A=12 at present): Green's function Monte Carlo (GFMC); virtually exact; limited to certain forms of interactions.

Highly accurate approximate solutions available for:

- Light nuclei (up to A=16 at present): No-core Shell model (NCSM); truncation in model space.
- Light and medium mass region (A=4, 16, 40 at present): Coupled cluster theory; truncation in model space and correlations.

☺ Theorists agree with each other

PHYSICAL REVIEW C, VOLUME 64, 044001

Benchmark test calculation of a four-nucleon bound state

H. Kamada,* A. Nogga, and W. Glöckle
Institut für Theoretische Physik II, Ruhr-Universität Bochum, D-44780 Bochum, Germany

E. Hiyama
High Energy Accelerator Research Organization, Institute of Particle and Nuclear Studies, Tsukuba 305-0801, Japan

M. Kamimura
Department of Physics, Kyushu University, Fukuoka 812-8581, Japan

K. Varga
Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37380
and Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen 4000, PO Box 51, Hunga

Y. Suzuki
Department of Physics, Niigata University, Niigata 950-2181, Japan

M. Viviani and A. Kievsky
INFN, Sezione di Pisa, I-56100 Pisa, Italy

S. Rosati
INFN, Sezione di Pisa, I-56100 Pisa, Italy
and Department of Physics, University of Pisa, I-56100 Pisa, Italy

J. Carlson
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

Steven C. Pieper and R. B. Wiringa
Physics Division, Argonne National Laboratory, Argonne, Illinois 60439

P. Navrátil
Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, California 94551
and Nuclear Physics Institute, Academy of Sciences of the Czech Republic, 250 68 Řež near Prague, Czech Republic

B. R. Barrett
Department of Physics, P.O. Box 210081, University of Arizona, Tucson, Arizona 85721

N. Barnea
The Racah Institute of Physics, The Hebrew University, 91904 Jerusalem, Israel

W. Leidemann and G. Orlandini
Dipartimento di Fisica and INFN (Gruppo Collegato di Trento), Università di Trento, I-38050 Povo, Italy

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In the past, several efficient methods have been developed to solve the Schrödinger equation for four-nucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's function Monte Carlo, the no-core shell model, and the effective interaction hyperspherical harmonic methods. In this article we compare the energy eigenvalue results and some wave function properties using the realistic *AV8'* *NN* interaction. The results of all schemes agree very well showing the high accuracy of our present ability to calculate the four-nucleon bound state.

TABLE I. The expectation values $\langle T \rangle$ and $\langle V \rangle$ of kinetic and potential energies, the binding energies E_b in MeV, and the radius in fm.

Method	$\langle T \rangle$	$\langle V \rangle$	E_b	$\sqrt{\langle r^2 \rangle}$
FY	102.39(5)	−128.33(10)	−25.94(5)	1.485(3)
CRCGV	102.30	−128.20	−25.90	1.482
SVM	102.35	−128.27	−25.92	1.486
HH	102.44	−128.34	−25.90(1)	1.483
GFMC	102.3(1.0)	−128.25(1.0)	−25.93(2)	1.490(5)
NCSM	103.35	−129.45	−25.80(20)	1.485
EIHH	100.8(9)	−126.7(9)	−25.944(10)	1.486

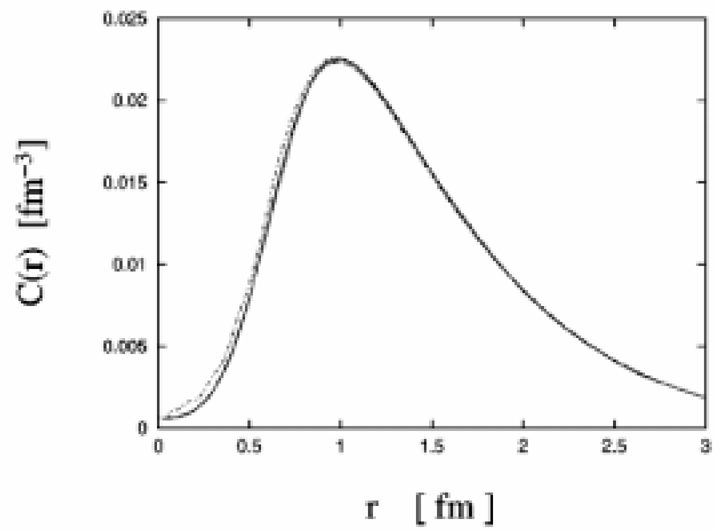


FIG. 1. Correlation functions in the different calculational schemes: EIHH (dashed-dotted curves), FY, CRCGV, SVM, HH, and NCSM (overlapping curves).

Working in a finite model space

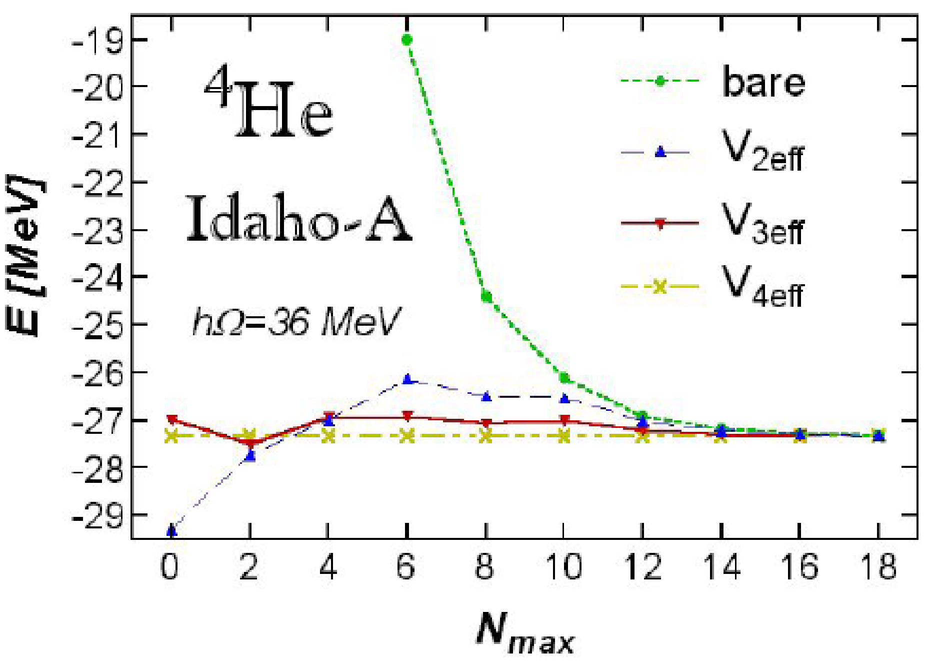
NCSM and Coupled-cluster theory solve the Schroedinger equation in a model space with a *finite* (albeit large) number of configurations or basis states.

Problem: High-momentum components of high-precision NN interactions require enormously large spaces.

Solution: Get rid of the high-momentum modes via a renormalization procedure. (Vlow-k is an example)

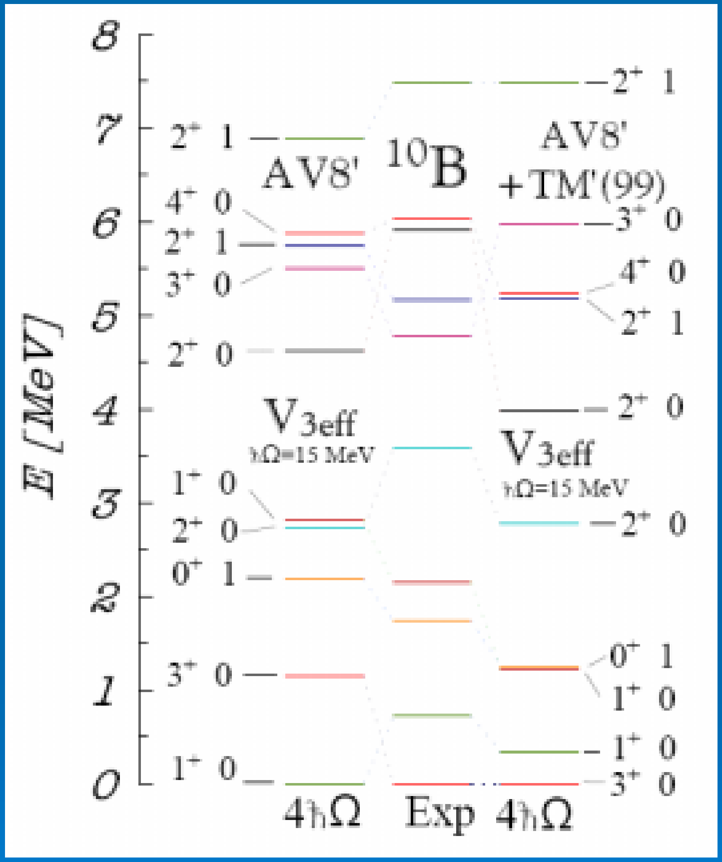
Price tag:

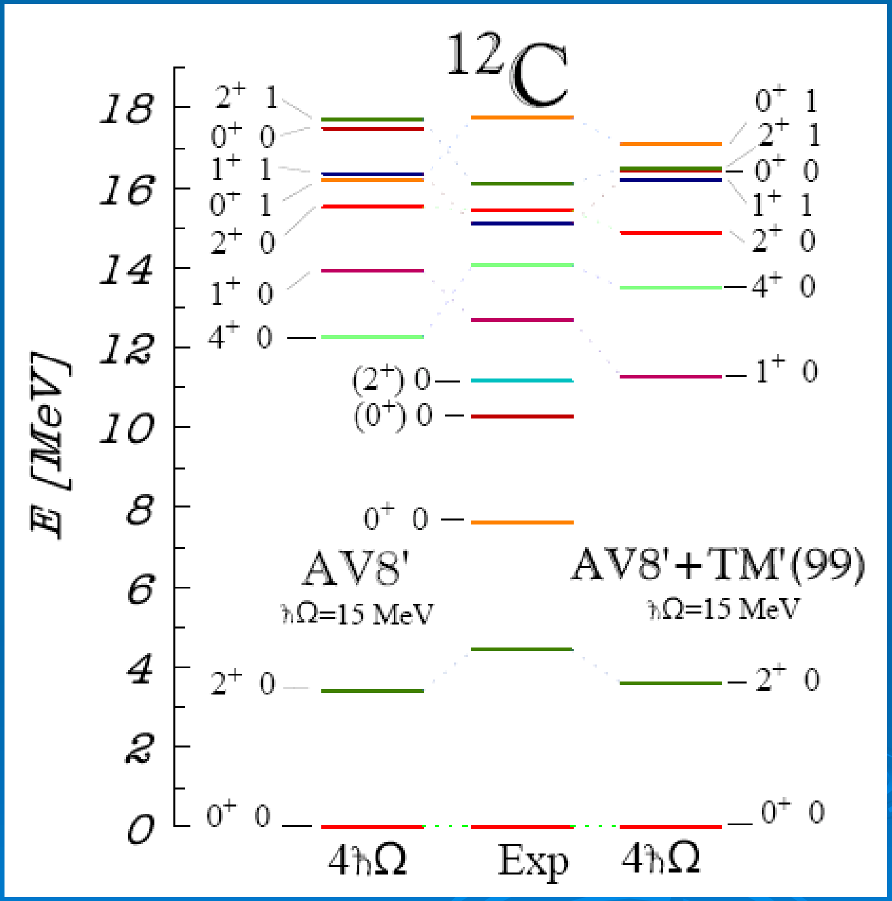
- Generation of 3, 4, …, A-body forces unavoidable.
- Observables other than the energy also need to be transformed.



E. Ormand
http://ww.phy.ornl.gov/npss03/ormand2.ppt

No-core Shell Model results for ^{10}B and ^{12}C





P. Navratil and W. E. Ormand, Phys. Rev. C68 (2003) 034305

No core shell model

Idea: Solve the A-body problem in a harmonic oscillator basis.

1. **Take K single particle orbitals**
2. **Construct a basis of Slater determinants**
3. **Express Hamiltonian in this basis**
4. **Find low-lying states via diagonalization**

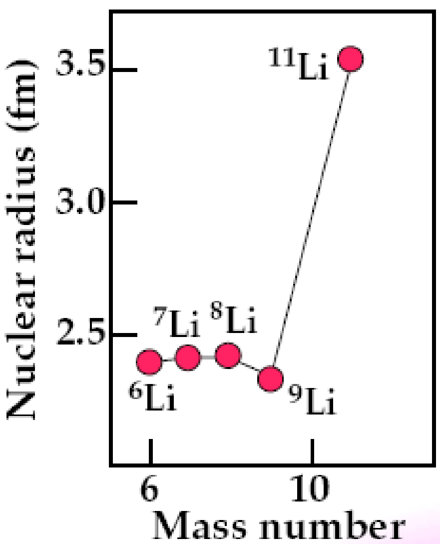
- ☺ **Get eigenstates and energies**
- ☺ **Symmetries like center-of-mass treated exactly**
- ☺ **No restrictions regarding Hamiltonian**

- ☹ **Number of configurations and resulting matrix very large: There are**

$$\binom{K}{A} = \frac{K!}{(K-A)!\,A!}$$

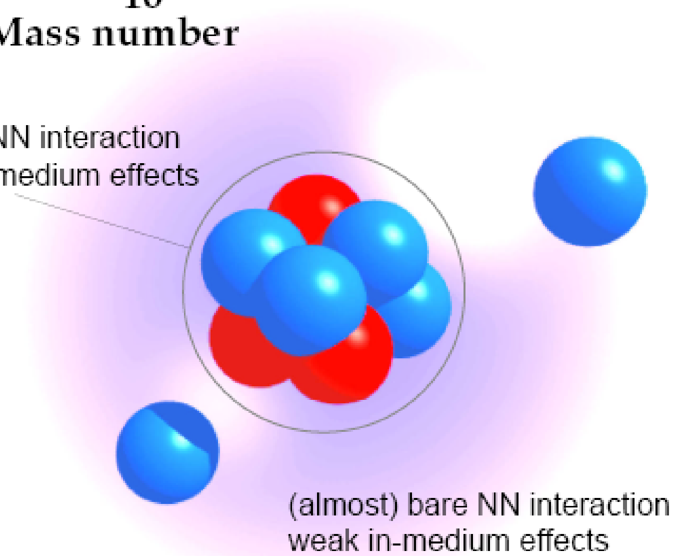
ways to distribute A nucleons over K single-particle orbitals.

Ab-initio calculations of charge radii of Li isotopes



I. Tanihata et al.
Phys. Rev. Lett. 55, 2676 (1985)

Interaction cross section measurements at Bevalac (790 MeV/u)



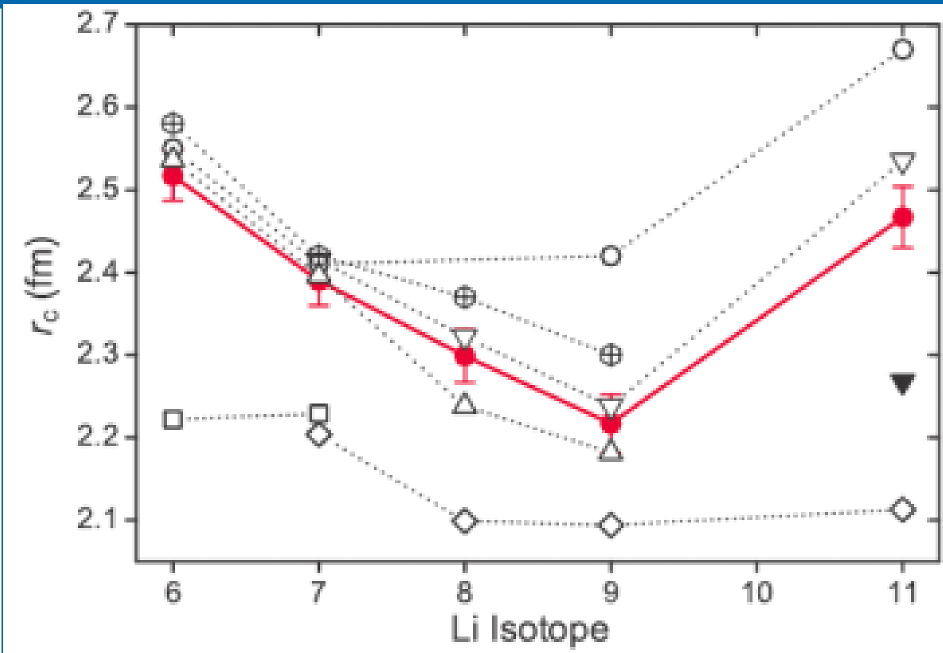


FIG. 2 (color online). Experimental charge radii of lithium isotopes (red, ●) compared with theoretical predictions: △: GFMC calculations [4,22], ▽: SVMC model [27,28] (▼: assuming a frozen ^{9}Li core), ⊕: FMD [26], ○: DCM [19], □ and ◇: *ab initio* NCSM [23,24].

R. Sanchez et al, PRL. 96 (2006) 33002.

N=8 results for ^{15}O, ^{17}O (G-matrix)

Diagonalize $\overline{H}$ (T's solved for n nucleons) in the $n \pm 1$ Fock space. $H \leftarrow T + V - \langle T_{cm} \rangle$

Gour et al in press PRC, 2006

BE/A

J^π	Expt.	N^{3}LO	CD-Bonn	AV18
^{15}O	7.46	6.64	7.58	5.25
^{16}O	7.98	7.4	8.33	5.90
^{17}O	7.75	7.17	8.03	5.62

^{17}O, all MeV

J^π	Expt.	N^{3}LO	CD-Bonn	AV18
$3/2^+$	5.085	5.68	6.41	3.946
$1/2^+$	0.870	-0.088	0.31	-0.390
$5/2^+$	0.0	0.0	0.0	0.0

^{15}O, all MeV

J^π	Expt.	N^{3}LO	CD-Bonn	AV18
$3/2^-$	6.176	6.26	7.35	4.452
$1/2^-$	0.0	0.0	0.0	0.0

A short history of coupled-cluster theory

Formal introduction:

1958: Coester, Nucl. Phys. 7, 421

1960: Coester and Kummel, Nucl. Phys. 17, 477

Introduction into Chemistry (late 60's):

1966: Cizek, J. Chem. Phys. 45, 4256 (1966); Adv. Chem. Phys. 14, 35 (1969)

1971: Cizek and Paldus, Int. J. Quantum Chem. 5, 359

Numerical implementations

1978: Pople et al., Int. J. Quantum Chem Symp, 14, 545

1978: Bartlett and Purvis, Int. J. Quantum Chem 14, 561

Initial nuclear calculations (1970's):

1978: Kummel, Luhrmann, Zabolitzky, Phys. Rep. 36, 1 and refs. therein

1980-90s: Bishop's group. Coordinate space.

Few applications in nuclei, explodes in chemistry and molecular sciences.

Hard-core interactions; computer power; unclear interactions

Nuclear physics reintroduction: ($1/E_{ph}$ expansion)

1999: Heisenberg and Mihiala, Phys. Rev. C59, 1440; PRL84, 1403 (2000)

Three nuclei; JJ coupled scheme; bare interactions, approximate V_{3N}

Useful References

Crawford and Schaefer, Reviews in Computational Chemistry, 14, 336 (2000)

Bartlett, Ann. Rev. Phys. Chem. 32, 359 (1981)

Coupled Cluster Theory: ab initio in medium mass nuclei

$$\left|\Psi\right\rangle = \exp\left(T\right)\left|\Phi\right\rangle$$

Correlated Ground-State wave function

Correlation operator

Reference Slater determinant

$$T = T_1 + T_2 + T_3 + \cdots$$

$$T_1 = \sum_{\substack{i<\varepsilon_f \\ a>\varepsilon_f}} t_{ai} a_a^{+} a_i$$

$$T_2 = \sum_{\substack{ij<\varepsilon_f \\ ab>\varepsilon_f}} t_{abij} a_a^{+} a_b^{+} a_j a_i$$

Energy

$$E = \left\langle\Phi\right|\exp(-T) H \exp\left(T\right)\left|\Phi\right\rangle$$

Amplitude equations

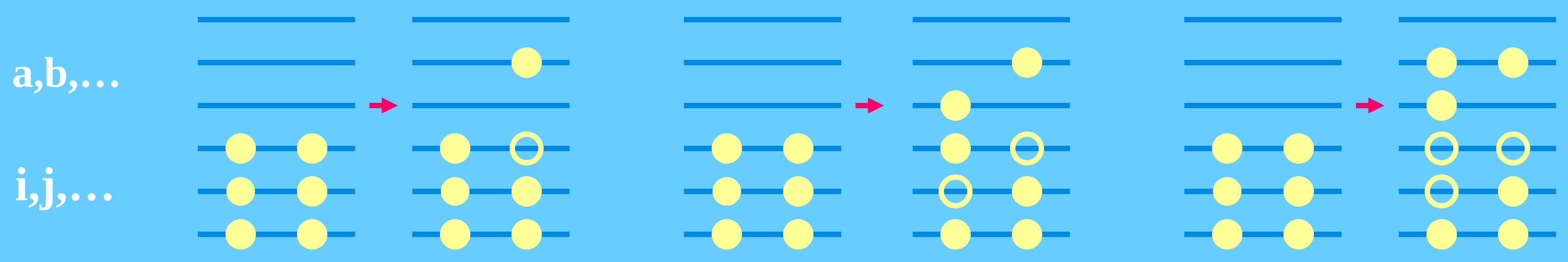
$$\left\langle\Phi_{ij\cdots}^{ab\cdots}\right|\exp(-T) H \exp\left(T\right)\left|\Phi\right\rangle = \left\langle\Phi_{ij\cdots}^{ab\cdots}\right|\overline{H}\left|\Phi\right\rangle = 0$$

- Nomenclature
  - Coupled-clusters in singles and doubles (CCSD)
  - …with triples corrections CCSD(T);

The many-body wave function in cluster amplitudes

$$\left|\Psi\right\rangle = e^{T^{(A)}}\left|\Phi\right\rangle, \quad T^{(A)} = \sum_{k=1}^{m_A} T_k$$

$$T_1 = \sum_{\substack{i\\a}} t_i^a \left|\Phi_i^a\right\rangle, \quad T_2 = \sum_{\substack{i>j\\a>b}} t_{ij}^{ab}\left|\Phi_{ij}^{ab}\right\rangle, \quad T_3 = \sum_{\substack{i>j>k\\a>b>c}} t_{ijk}^{abc}\left|\Phi_{ijk}^{abc}\right\rangle$$



$m_A = N$, exact theory;

$m_A < N$, approximate theory

$m_A = 2 \quad T = T_1 + T_2 \qquad CCSD \qquad n_o^2 n_u^4 \left(n_o^2 n_u^2\right)$

$m_A = 3 \quad T = T_1 + T_2 + T_3 \qquad CCSDT \qquad n_o^3 n_u^5 \left(n_o^3 n_u^3\right)$

View of the CC equations from 10,000 feet

$$He^{T}|\Phi\rangle = E_0 e^{T}|\Phi\rangle$$

$$e^{-T}He^{T}|\Phi\rangle = E_0 e^{-T}e^{T}|\Phi\rangle = E_0|\Phi\rangle = \overline{H}|\Phi\rangle$$

$$\overline{H} = e^{-T}He^{T} = \left(He^{T}\right)_C$$

$$\overline{H} = H + [H,T] + \frac{1}{2}[[H,T],T] + \frac{1}{6}[[[H,T],T],T] + \frac{1}{24}[[[[H,T],T],T],T]$$

Finite series in T.

$$\left\langle \Phi^{a_1 a_2 \ldots a_k}_{i_1 i_2 \ldots i_k} \middle| \left(H_N e^{T^{(A)}}\right)_C \middle| \Phi \right\rangle = 0, \quad k = 1,\ldots,m_A$$

$$E_0 = \langle \Phi | H | \Phi \rangle + \left\langle \Phi \middle| \left(H_N e^{T^{(A)}}\right)_C \middle| \Phi \right\rangle = \left\langle \Phi \middle| \left[H_N \left(T_1 + T_2 + \frac{1}{2}T_1^2 \right) \right]_C \middle| \Phi \right\rangle$$

Derivation of CC equations

T_1 amplitudes from: $\left\langle \Phi_i^a \middle| \exp(-T) H \exp(T) \middle| \Phi \right\rangle = 0$

$$
\begin{aligned}
0 \;=\;& f_{ai} + \sum_c f_{ac} t_i^c - \sum_k f_{ki} t_k^a + \sum_{kc} \langle ka||ci\rangle t_k^c + \sum_{kc} f_{kc} t_{ik}^{ac} + \frac{1}{2}\sum_{kcd} \langle ka||cd\rangle t_{ki}^{cd} - \\
& \frac{1}{2}\sum_{klc} \langle kl||ci\rangle t_{kl}^{ca} - \sum_{kc} f_{kc} t_i^c t_k^a - \sum_{klc} \langle kl||ci\rangle t_k^c t_l^a + \sum_{kcd} \langle ka||cd\rangle t_k^c t_i^d - \qquad [152] \\
& \sum_{klcd} \langle kl||cd\rangle t_k^c t_i^d t_l^a + \sum_{klcd} \langle kl||cd\rangle t_k^c t_{li}^{da} - \frac{1}{2}\sum_{klcd} \langle kl||cd\rangle t_{ki}^{cd} t_l^a - \frac{1}{2}\sum_{klcd} \langle kl||cd\rangle t_{kl}^{ca} t_i^d ,
\end{aligned}
$$

Note T_2 amplitudes also come into the equation.

T_2 amplitudes from: $\left\langle \Phi_{ij}^{ab} \middle| \exp(-T) H \exp(T) \middle| \Phi \right\rangle = 0$

$$
\begin{aligned}
0 \;=\;& \langle ab||ij\rangle + \sum_c \left(f_{bc} t_{ij}^{ac} - f_{ac} t_{ij}^{bc} \right) - \sum_k \left(f_{kj} t_{ik}^{ab} - f_{ki} t_{jk}^{ab} \right) + \qquad [153] \\
& \frac{1}{2} \sum_{kl} \langle kl||ij\rangle t_{kl}^{ab} + \frac{1}{2} \sum_{cd} \langle ab||cd\rangle t_{ij}^{cd} + P(ij)P(ab) \sum_{kc} \langle kb||cj\rangle t_{ik}^{ac} + \\
& P(ij) \sum_c \langle ab||cj\rangle t_i^c - P(ab) \sum_k \langle kb||ij\rangle t_k^a + \\
& \frac{1}{2} P(ij)P(ab) \sum_{klcd} \langle kl||cd\rangle t_{ik}^{ac} t_{lj}^{db} + \frac{1}{4} \sum_{klcd} \langle kl||cd\rangle t_{ij}^{cd} t_{kl}^{ab} - \\
& P(ab) \frac{1}{2} \sum_{klcd} \langle kl||cd\rangle t_{ij}^{ac} t_{kl}^{bd} - P(ij) \frac{1}{2} \sum_{klcd} \langle kl||cd\rangle t_{ik}^{ab} t_{jl}^{cd} + \\
& P(ab) \frac{1}{2} \sum_{kl} \langle kl||ij\rangle t_k^a t_l^b + P(ij) \frac{1}{2} \sum_{cd} \langle ab||cd\rangle t_i^c t_j^d - P(ij)P(ab) \sum_{kc} \langle kb||ic\rangle t_k^a t_j^c + \\
& P(ab) \sum_{kc} f_{kc} t_k^a t_{ij}^{bc} + P(ij) \sum_{kc} f_{kc} t_i^c t_{jk}^{ab} - \\
& P(ij) \sum_{klc} \langle kl||ci\rangle t_k^c t_{lj}^{ab} + P(ab) \sum_{kcd} \langle ka||cd\rangle t_k^c t_{ij}^{db} + \\
& P(ij)P(ab) \sum_{kcd} \langle ak||dc\rangle t_i^d t_{jk}^{bc} + P(ij)P(ab) \sum_{klc} \langle kl||ic\rangle t_l^a t_{jk}^{bc} + \\
& P(ij) \frac{1}{2} \sum_{klc} \langle kl||cj\rangle t_i^c t_{kl}^{ab} - P(ab) \frac{1}{2} \sum_{kcd} \langle kb||cd\rangle t_k^a t_{ij}^{cd} - \\
& P(ij)P(ab) \frac{1}{2} \sum_{kcd} \langle kb||cd\rangle t_i^c t_k^a t_j^d + P(ij)P(ab) \frac{1}{2} \sum_{klc} \langle kl||cj\rangle t_i^c t_k^a t_l^b - \\
& P(ij) \sum_{klcd} \langle kl||cd\rangle t_k^c t_i^d t_{lj}^{ab} - P(ab) \sum_{klcd} \langle kl||cd\rangle t_k^c t_l^a t_{ij}^{db} + \\
& P(ij) \frac{1}{4} \sum_{klcd} \langle kl||cd\rangle t_i^c t_j^d t_{kl}^{ab} + P(ab) \frac{1}{4} \sum_{klcd} \langle kl||cd\rangle t_k^a t_l^b t_{ij}^{cd} + \\
& P(ij)P(ab) \sum_{klcd} \langle kl||cd\rangle t_i^c t_l^b t_{kj}^{ad} + P(ij)P(ab) \frac{1}{4} \sum_{klcd} \langle kl||cd\rangle t_i^c t_k^a t_j^d t_l^b .
\end{aligned}
$$

Nonlinear terms in t2 (4th order)

$$P(ij)\, f(ij) = f(ij) - f(ji)$$

An interesting mess.
But solvable….

Diagonalization: configuration-interaction, interacting shell model

Yields eigenfunctions which are linear combinations of particle-hole amplitudes

$$\left|\Psi_\alpha\right\rangle = \left(b^\alpha + b^\alpha_{ai} a^+_a a_i + b^\alpha_{abij} a^+_a a^+_b a_i a_j + \cdots\right)\left|\Phi_0\right\rangle$$

1p-1h

2p-2h

“Mean field”

Hamiltonian diagonalization (Barrett et al.)

- **Detailed spectroscopic information available**
- **Wave functions calculated and stored**
- **Dimension of problem increases dramatically with the number of active particles (combinatorial growth).**
- **Disconnected diagrams enter if truncated**

Relationship between shell model and CC amplitudes

$$B_1 = T_1$$

$$B_2 = T_2 + \frac{1}{2}T_1^2$$

$$B_3 = T_3 + T_2T_1 + \frac{1}{6}T_1^3$$

$$B_4 = T_4 + T_3T_1 + \frac{1}{2}T_2^2 + \frac{1}{2}T_2T_1^2 + \frac{1}{24}T_1^4$$

$\ldots$

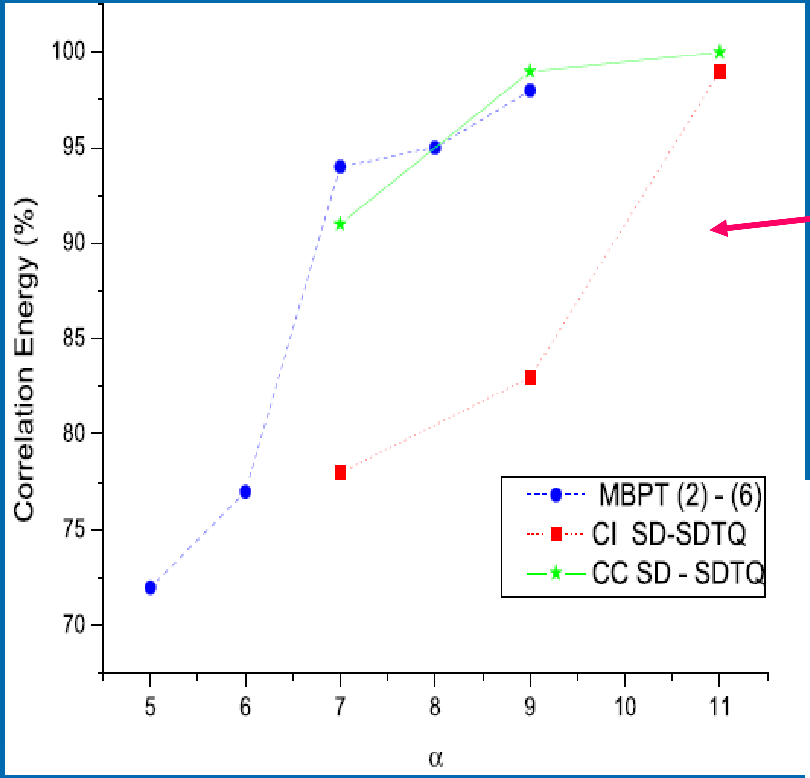
CCSD

CR-CCSD(T)

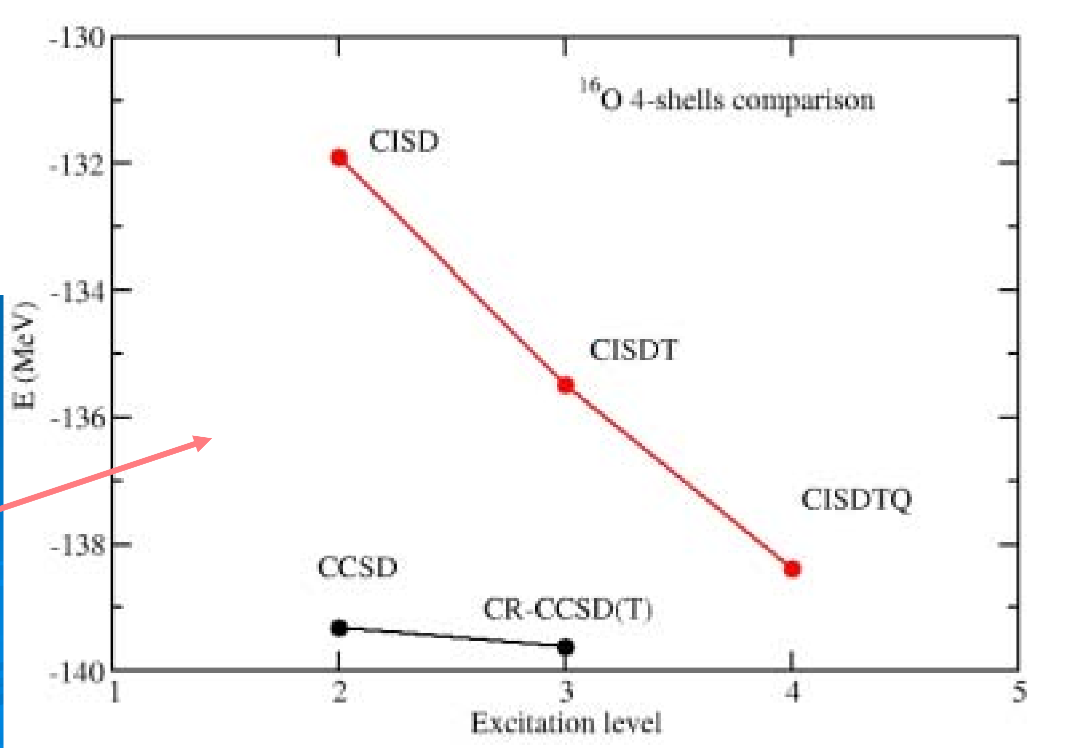
“Disconnected quadruples”

“Connected quadruples”

Comparisons with other many-body techniques

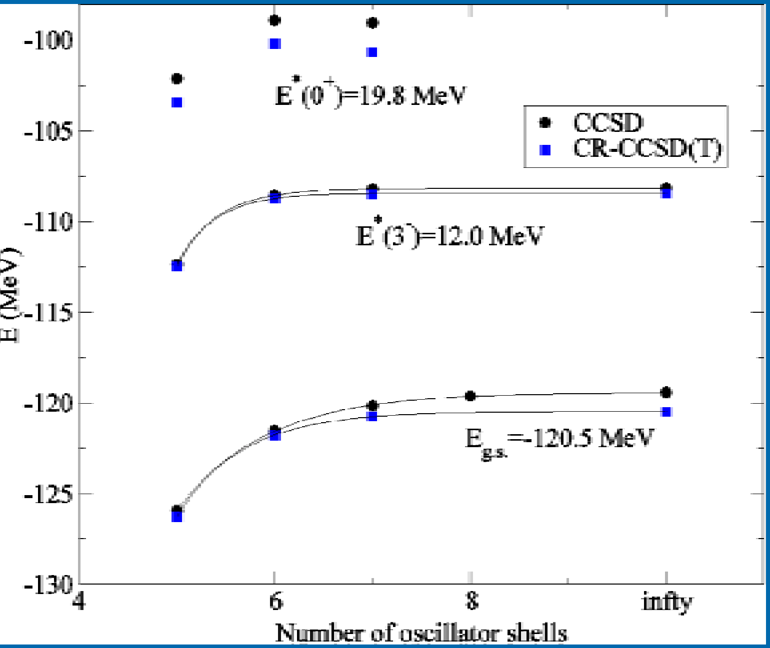


Quantum chemistry example (Bartlett et al)



Nuclear Example (Kowalski et al PRL 2004).

What about the first excited 3-?



From experiment

$$\Delta\varepsilon_\pi = \varepsilon_\pi(0d_{5/2}) - \varepsilon_\pi(0p_{1/2})$$
$$= \left[\mathrm{BE}(^{16}O) - \mathrm{BE}(^{17}F)\right] + \left[\mathrm{BE}(^{16}O) - \mathrm{BE}(^{15}N)\right]$$
$$= 11.526\ \mathrm{MeV}$$

$$\Delta\varepsilon_\nu = \varepsilon_\nu(0d_{5/2}) - \varepsilon_\nu(0p_{1/2})$$
$$= \left[\mathrm{BE}(^{16}O) - \mathrm{BE}(^{17}O)\right] + \left[\mathrm{BE}(^{16}O) - \mathrm{BE}(^{15}O)\right]$$
$$= 11.521\ \mathrm{MeV}$$

Interactions among nucleons lowers by about 11.5-6.1=5.4 MeV

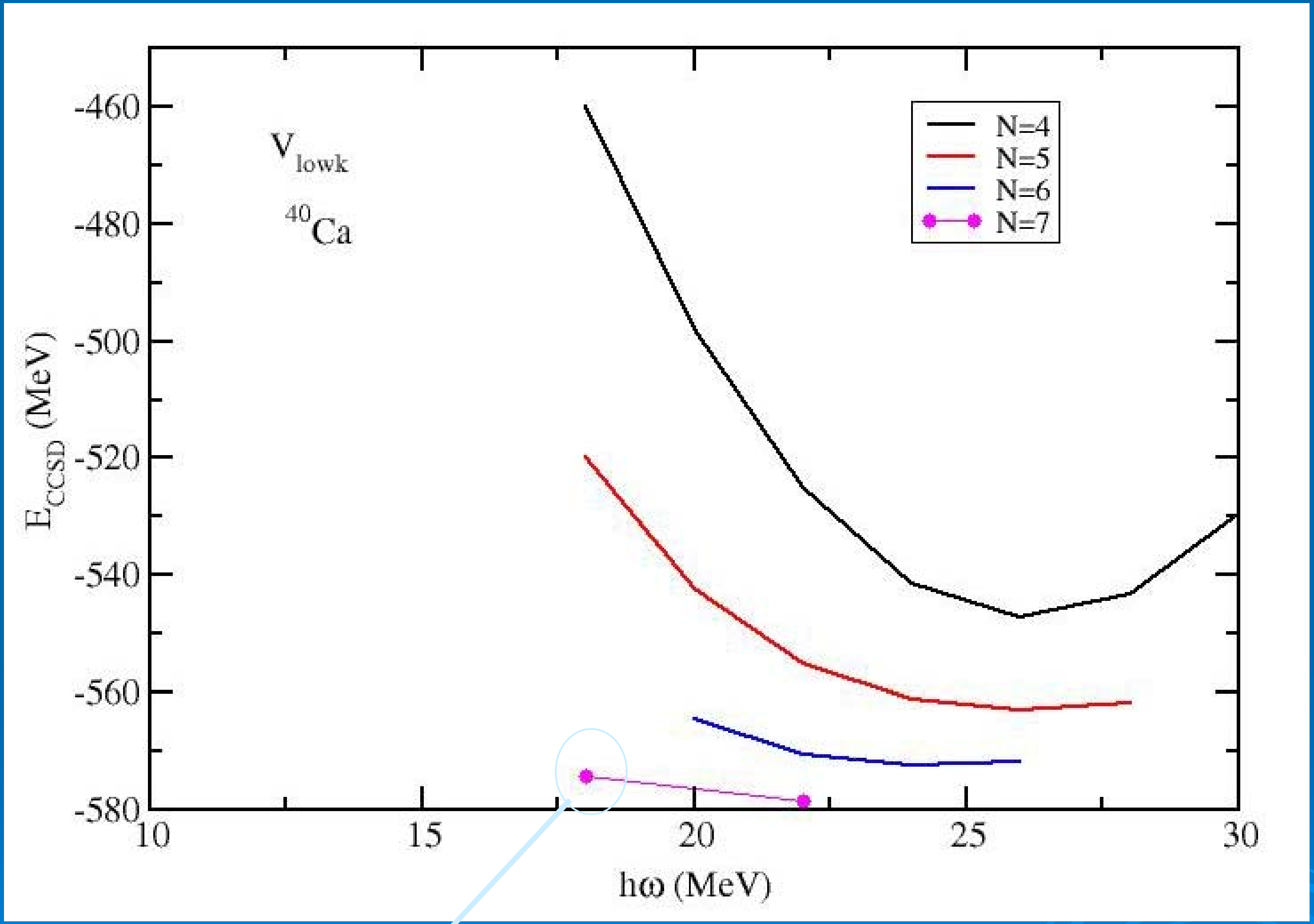
From CCSD

$$\Delta\varepsilon_\pi = 15.846\ \mathrm{MeV}$$
$$\Delta\varepsilon_\nu = 15.789\ \mathrm{MeV}$$

Interactions among nucleons lowers by about 15.8-11.5=4.3 MeV

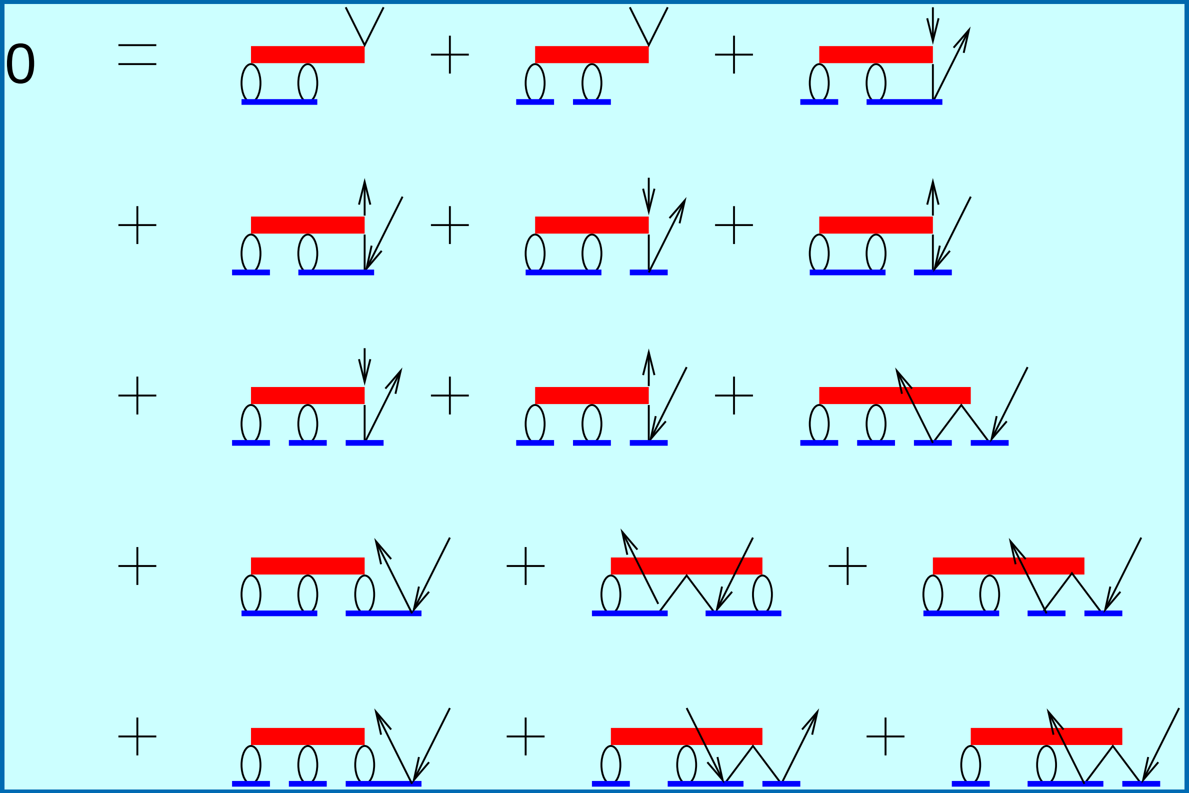
Much of the discrepancy comes from where the interaction places the 0p shell relative to the 0d1s shell.

Ca40: the next frontier (no com corrections)



4.2 TFlop-hours at NERSC

Inclusion of three-body forces:



Calculations with three-body forces are underway

Initial V3-CCSD results
(proof of principle, Papenbrock, Hagen, et al)

$$E = \langle \Phi | \exp(-T)(H = T - T_{cm} + V_2 + V_3)\exp(T) | \Phi \rangle$$

V_2 is Vlowk of AV18 at λ=1.9 fm^{-1}
Nogga, Bogner, Schwenk adjustment of V_3 from EFT (N^2LO) adjusted for ^4He (mixed bag, I know). Considering only T=1/2+ so far).

(1): V2 only
(2): (1)+v3 normal ordered contribution to vacuum energy
(3): (1)+(2)+ v3 contribution to CCSD energy
(4): (1)+(2)+(3)+ v3 normal ordered contribution to one-body operator
(5): (1)+(2)+(3)+(4)+ v3 normal ordered contribution to two-body operator
(6): (1)+(2)+(3)+(4)+(5)+ t1 and t2 amplitudes consistently calculated with v3

	(1)	(2)	(3)	(4)	(5)	(6)
4He,N=3	-22.957	-22.442	-22.443	-22.523	-22.525	-22.523
4He, N=4	-25.822	-25.306	-25.307	-25.402	-25.384	-25.387
16O, N=3	-124.389	-118.199	-118.208	-118.862	-118.872	-118.877
16O, N=4	-140.896	-134.707	-134.710	-136.038	-135.891	-135.930

Rigged Hilbert space formulation : Gamow Shell Model (2002)

$$\hat{H}\Psi = \left(e - i\frac{\Gamma}{2}\right)\Psi \; : \qquad \Psi(0,k)=0 \;,\quad \Psi(\vec{r},k) \xrightarrow[r\to\infty]{} O_l(kr)$$

outgoing solution

Eigenvalues : $k_n = \sqrt{\frac{2m}{\hbar^2}\left(e_n - i\frac{\Gamma_n}{2}\right)}$ are the poles of the S-matrix :
- Bound states $(k_n = i\kappa_n)$
- Antibound states $(k_n = -i\kappa_n)$
- Resonances $(k_n = \pm\gamma_n - i\kappa_n)$

Completness relation for one-body states:

(T.Berggren (1968))

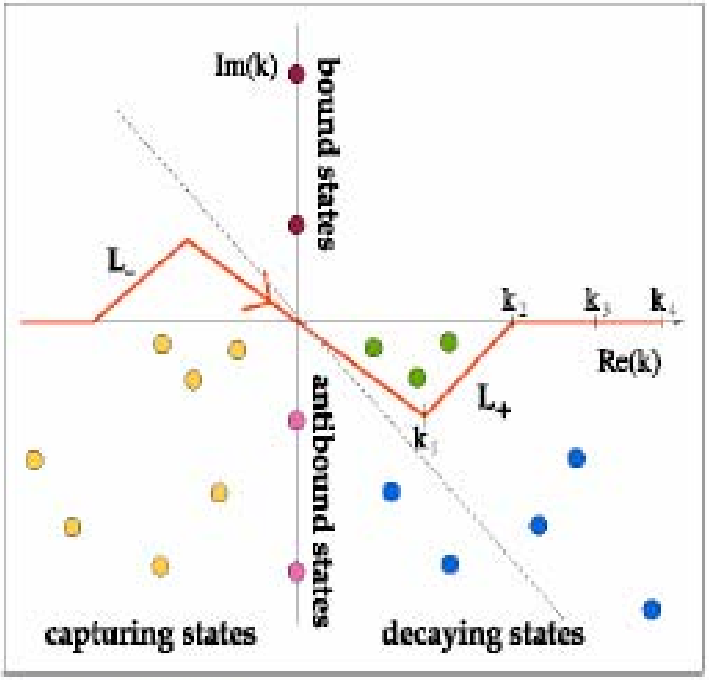
$$\sum_n |u_n\rangle\langle\tilde{u}_n| + \int_{L+} |u_k\rangle\langle\tilde{u}_k| dk = 1$$

bound, anti-bound, and resonance states

non-resonant continuum

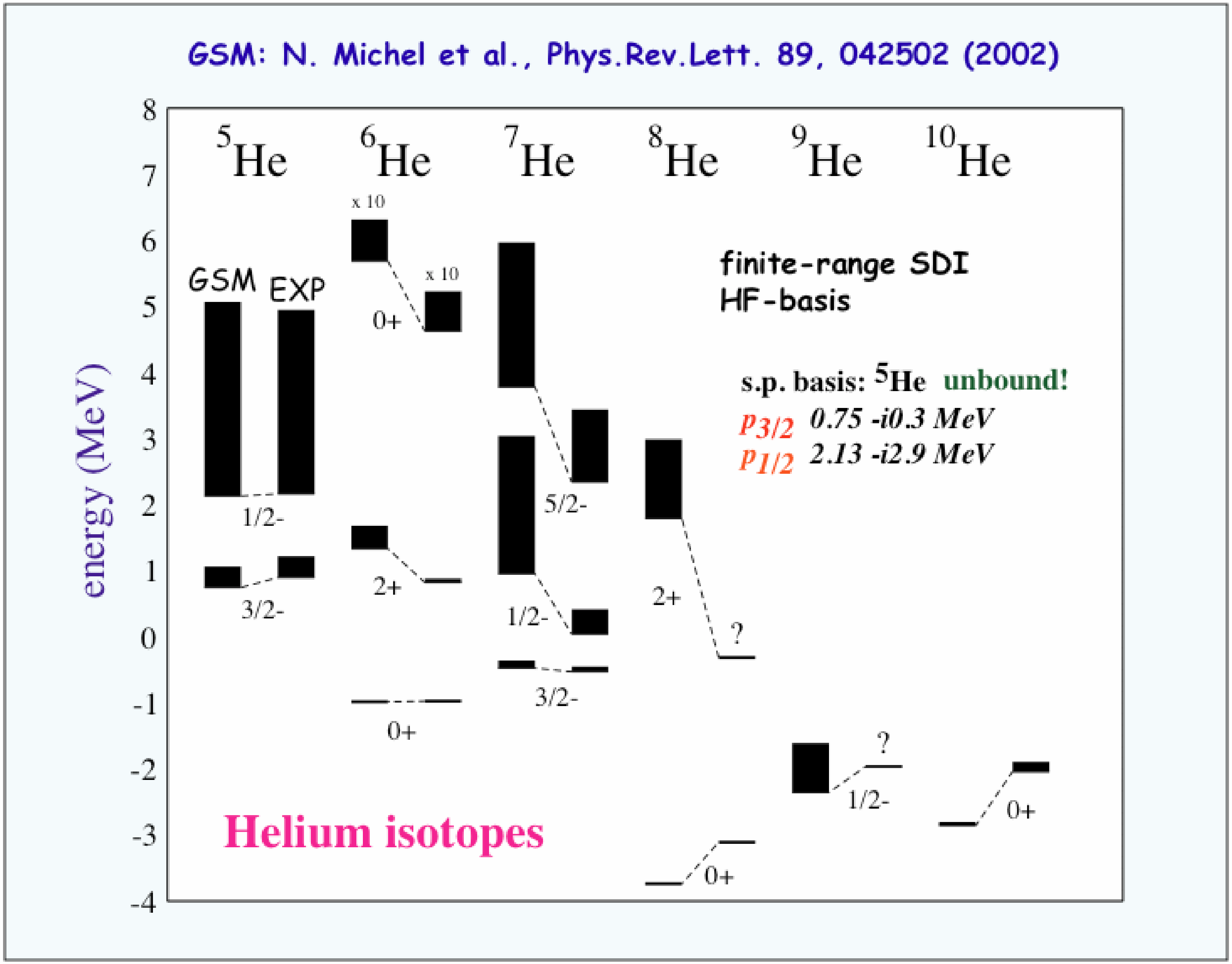
$$\sum_n |u_n\rangle\langle\tilde{u}_n| + \sum_{i=1}^{Nd} |u_i\rangle\langle\tilde{u}_i| \cong 1 \; ; \quad \langle u_i|\tilde{u}_j\rangle = \delta_{ij}$$

$$\sum_k |SD_k\rangle\langle SD_k| \cong 1$$



complex-symmetric eigenvalue problem for hermitian Hamiltonian

Ploszajczak et al.

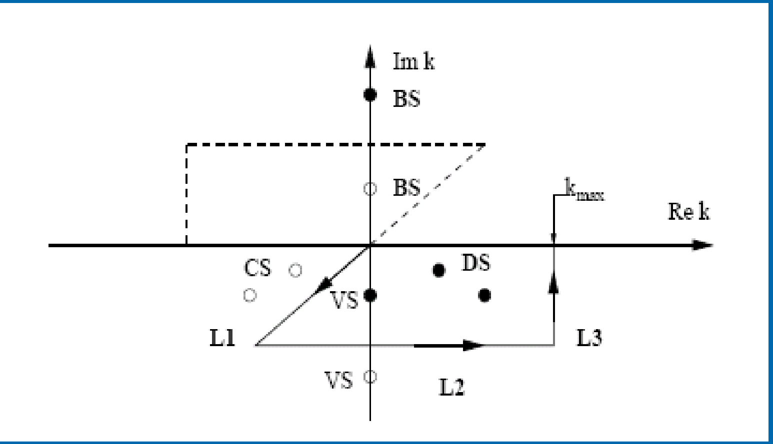

GSM: N. Michel et al., Phys.Rev.Lett. 89, 042502 (2002)
energy (MeV)
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
5He
6He
7He
8He
9He
10He
GSM
EXP
1/2-
3/2-
x 10
x 10
0+
2+
0+
5/2-
1/2-
3/2-
2+
?
0+
?
1/2-
0+
finite-range SDI
HF-basis
s.p. basis: 5He unbound!
p3/2 0.75 -i0.3 MeV
p1/2 2.13 -i2.9 MeV
Helium isotopes

Gamow-Hartree-Fock basis

The self-consistent Hartree-Fock potential in a plane wave-basis gives an integral equation for the single-particle states.

$$\frac{\hbar^2}{m_{\text{eff}}} k^2 \psi_{nlj}(k) + \int_{L^+} dk' k'^2 V_{HF}(jlkk') \psi_{nl}(k') = E_{nl} \psi_{nl}(k)$$

Analytically continue the momentum space Schrödinger equation in the complex k-plane by deforming the integration contour.



The Hartree-Fock states forms a complete bi-orthogonal basis:

$$1 = \sum_{n \in C} |\psi_{nl}\rangle\langle\psi^*_{nl}| + \int_{L^+} dk k^2 |\psi_l(k)\rangle\langle\psi^*_l(k)|.$$

A discrete sum over bound and resonant states and an integral over the non-resonant continuum.

Discretizing the continuum integral yields a finite complete basis within the discretization space

$$1 = \sum_{n}^{N} |\psi_{nl}\rangle\langle\psi^*_{nl}| = \sum_{n}^{N}\sum_{i=1}^{N} \psi_{nl}(i)\psi_{nl}(i).$$

Complex CCSD for the He chain
[Preliminary, G. Hagen et al.]

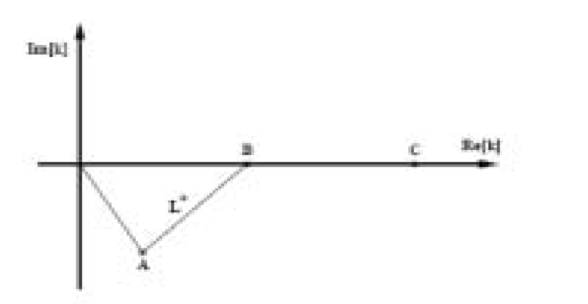
- Very low neutron separation energy. p-orbits are the main decay channel and build up the main part of the halo densities.
- Protons have large separation energies (20-30 MeV), mainly occupying deeply bound s-orbits.

Neutron orbitals are Gamow states for s-p partial waves and oscillators for higher partial waves (d-g).

Neutrons
15s1/2
15p3/2
15p1/2
4d5/2
4d3/2
…

Proton orbitals are Oscillators restricted by N=10 major shells and lmax

Protons
5s1/2
4p3/2
4p1/2
4d5/2
4d3/2
…



	$\Lambda = 1.8\text{fm}^{-1}$		$\Lambda = 1.9\text{fm}^{-1}$		$\Lambda = 2.0\text{fm}^{-1}$		Expt.	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
$s_{1/2}$	-18.678	0.000	-17.452	0.000	-16.021	0.000	-20.578	0.000
$p_{3/2}$	1.465	-0.954	1.609	-1.141	1.765	-1.347	0.890	-0.324
$p_{1/2}$	2.376	-3.081	2.389	-3.192	2.488	-3.388	2.160	-2.785

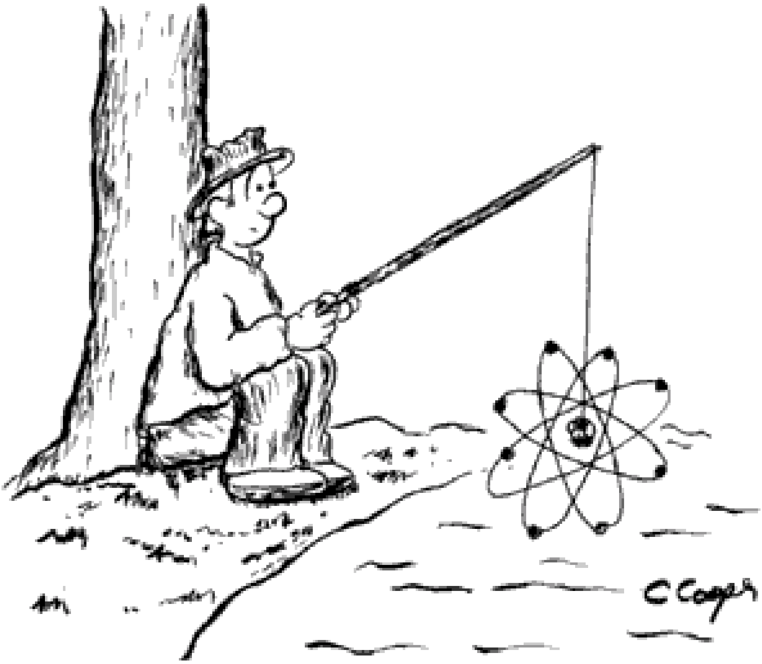
CCSD calculation of the 4-10He ground states with the low-momentum N3LO NN interaction (L=1.9 fm-1) for increasing number of partial waves. The energies E are in MeV for both real and imaginary parts (Hagen et al. in prep).

	^{4}He		^{5}He		^{6}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
s – p	-24.92	0.00	-20.08	-0.54	-18.02	-0.44
s – d	-26.58	0.00	-23.45	-0.23		
s – f	-27.57	0.00				
Expt.	-28.30	0.00	-27.41	-0.33	-29.27	0.00

	^{7}He		^{8}He		^{9}He		^{10}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
s – p	-17.02	-0.24	-16.97	-0.00	-15.28	-0.40	-13.82	-0.12
s – f			-28.98	-0.00				
Expt.	-28.82	-0.15	-31.41	0.00	-30.26	-0.1?	-30.34	?

Perspectives on CC methods in nuclear physics

- Developing CC for nuclei requires simultaneous developments for the effective interaction
- We have extensive calculations for ^{16}O:
  - CCSD ground and excited states
  - CR-CCSD(T) ground and excited states
  - A+/-1 calculations
- New stuff:
  - Coupled-clusters in the continuum (reactions)
  - Three-body force (proof of principle)
    - Future steps: Higher-Order SVD for compression
  - Gearing up for ^{40}Ca.
- CC theory represents a way to move to heavier nuclei.
- CC is computationally intensive; algorithm development to move further (9-10 shells, mass 100) is also underway



Nuclear Fishin'

"Chance is always powerful. Let your hook be always cast; in the pool where you least expect it, there will be a fish."
-- Ovid (43 BC – 17 AD)

Recall Hartree-Fock II

Putting it all together

$$\delta E = \frac{-\hbar^2\nabla^2}{2m}\psi_\kappa(\vec{r}\,') + \sum_\beta \int d\vec{r}_2 \psi^*_\beta(\vec{r}_2) V(\vec{r}\,',\vec{r}_2)\psi_\kappa(\vec{r}\,')\psi_\beta(\vec{r}_2) - \sum_\alpha \int d\vec{r}_2 \psi^*_\alpha(\vec{r}_2) V(\vec{r}\,',\vec{r}_2)\psi_\alpha(\vec{r}\,')\psi_\kappa(\vec{r}_2)$$

$$\rho(\vec{r}) = \sum_\alpha \psi^*_\alpha(\vec{r})\psi_\alpha(\vec{r}) \qquad \rho(\vec{r},\vec{r}\,') = \sum_\alpha \psi^*_\alpha(\vec{r})\psi_\alpha(\vec{r}\,')$$

$$\frac{-\hbar^2\nabla^2}{2m}\psi_\kappa(\vec{r}\,') + \int d\vec{r}_2 \rho(\vec{r}_2) V(\vec{r}\,',\vec{r}_2)\psi_\kappa(\vec{r}\,') - \int d\vec{r}_2 \rho(\vec{r}_2,\vec{r}\,') V(\vec{r}\,',\vec{r}_2)\psi_\kappa(\vec{r}_2) = e_\kappa \psi_\kappa(\vec{r})$$

Direct term (easy)

Exchange term (hard)

$$\left[\frac{-\hbar^2\nabla^2}{2m} + \rho(\vec{r}\,')\right]\psi_\kappa(\vec{r}\,') - \int d\vec{r}_2 \rho(\vec{r}\,',\vec{r}_2)\psi_\kappa(\vec{r}_2) = e_\kappa \psi_\kappa(\vec{r})$$

A digression to something called Skyrme Hartree-Fock

$$\rho(\vec{r}_1,\vec{r}_2)=\delta(\vec{r}_1-\vec{r}_2)\rho(\vec{r}_1)$$

Keep everything local

$$\mathrm{E}[\rho,\tau,\vec{J}]=\frac{1}{2M}\tau+\frac{3}{8}t_0\rho^2+\frac{1}{16}t_3\rho^{2+\alpha}+\frac{1}{16}(3t_1+5t_2)\rho\tau$$
$$+\frac{1}{64}(9t_1-5t_2)(\nabla\rho)^2-\frac{3}{4}W_0\rho\nabla\bullet\vec{J}+\frac{1}{32}(t_1-t_2)\vec{J}^2$$

SKIII

$$t_0=-1129,\ t_1=395,$$
$$t_2=-95,\ t_3=14000,\ W_0=120$$

$$\rho(\vec{r})=\sum_i|\psi_i(\vec{r})|^2 \qquad \tau(\vec{r})=\sum_i|\nabla\psi_i(\vec{r})|^2$$

$$\text{Minimize}: \quad \mathrm{E}=\int d\vec{r}E[\rho,\tau,J]$$

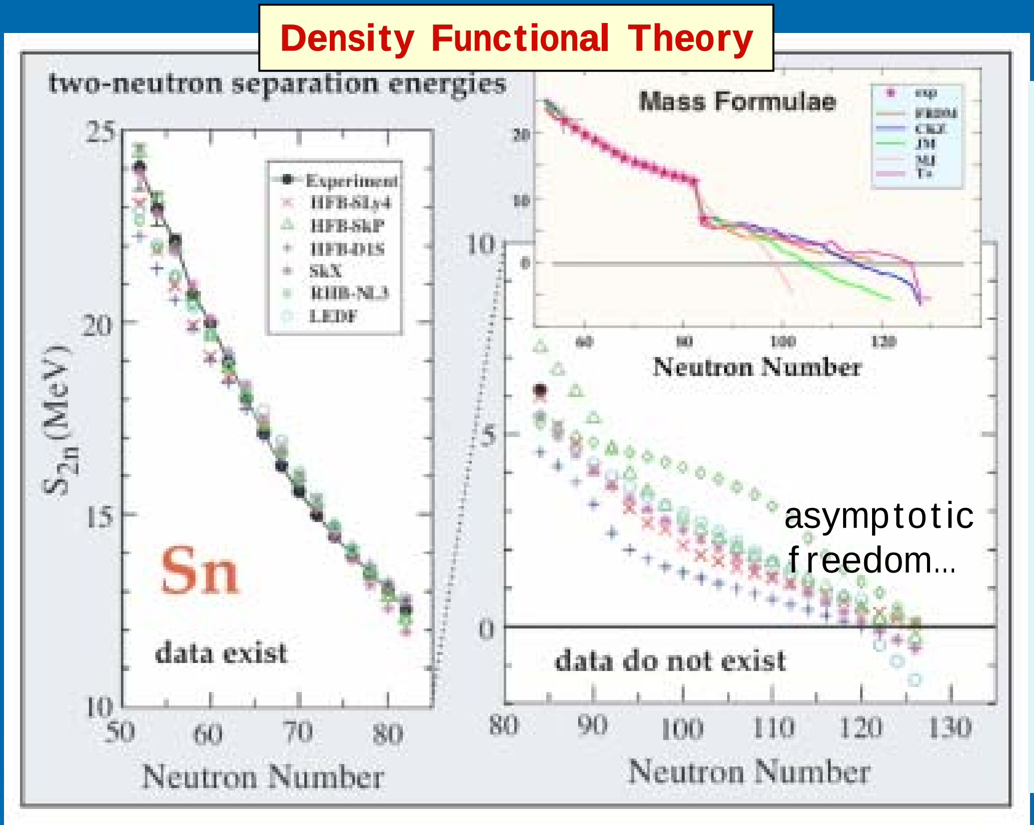
$$\left(-\nabla\frac{1}{2M^*(\vec{r})}\nabla+U(\vec{r})+\frac{3}{4}W_0\nabla\rho\bullet\frac{1}{i}\nabla\times\sigma\right)\psi_\alpha(\vec{r})=\varepsilon_\alpha\psi_\alpha(\vec{r})$$

$$\frac{1}{2M^*(\vec{r})}=\frac{1}{2M}+\left[\frac{3}{16}t_1+\frac{5}{16}t_2\right]\rho(\vec{r})$$

The ratio of Skyrm forces (parameterizations) to the number of nuclei is about the same as the number of lawyers to citizens in the U.S.

Can we be more systematic??

The mean field picture of the nucleus



This is Nuclear DFT (not HF from the initial NN interaction) – "HFB".

Nuclear DFT functionals (Skyrme) predict different behaviors near the drip lines. Which one is correct?

Can we include further density operators in energy density functional?

Can we use the unitary limit to constrain the form of the potential?

Challenge: Find the appropriate energy density functional that describes nuclei (Find connection to the ab initio potentials)

Homework problem: Take some psudo-data (e.g. from John Clark's neural network) for Sn132-140 (and maybe a few other select chains). Get DFT fits. Do you still have asymptotic freedom?? When can we stop?

Microscopic Mass Formula

(can we go below 500 keV?)

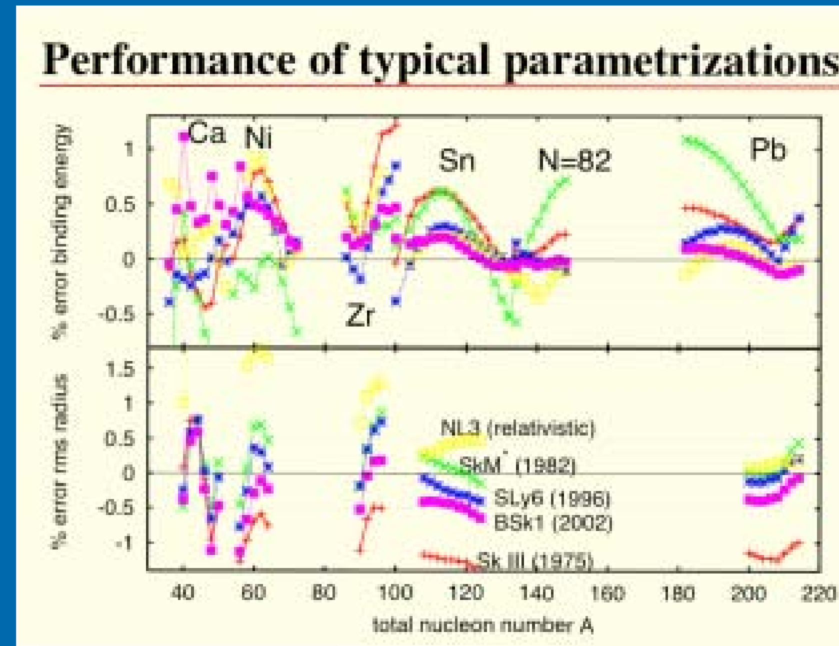
Goriely, ENAM'04

Reinhard 2004

HFB models: weapons of mass production

Recent improvements of HFB mass formulas	Accuracy σ_{rms} (2149 nuc)
HFB-2 masses: M^*_s=1.04, vol. pairing	659 keV
HFB-3 masses: M^*_s=1.12, vol+surf pairing	635 keV
HFB-7 masses: M^*_s=0.80, vol+surf pairing	657 keV
HFB-8 masses: M^*_s=0.80, vol. pairing, PLN (part.nb proj.)	635 keV
HFB-9 masses: M^*_s=0.80, vol. pairing, PLN, J=30MeV	733 keV

Constrained on both Nuclei and Infinite Nuclear Matter for astrophysics applications

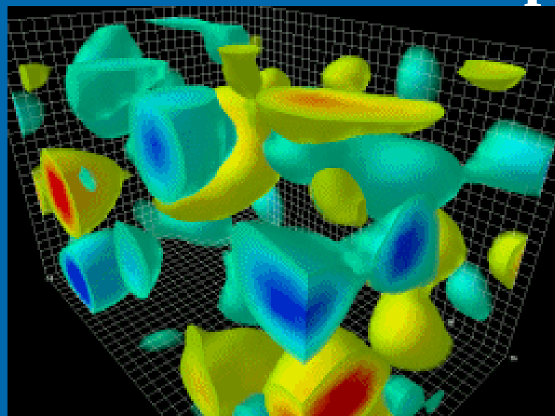


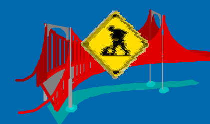
Challenges:

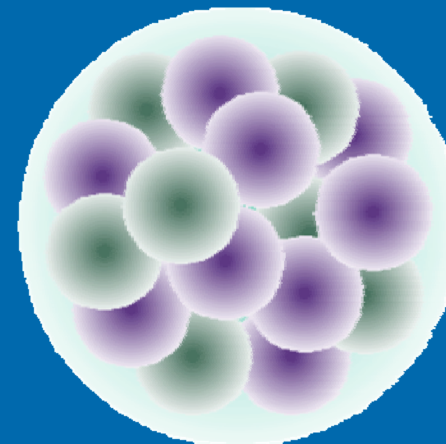
- need for error and covariance analysis (theoretical error bars in unknown regions)
- a number of observables need to be considered (masses, radii, collective modes)
- only data for selected nuclei used

Philosophical issue: What are the relevant degrees of freedom?

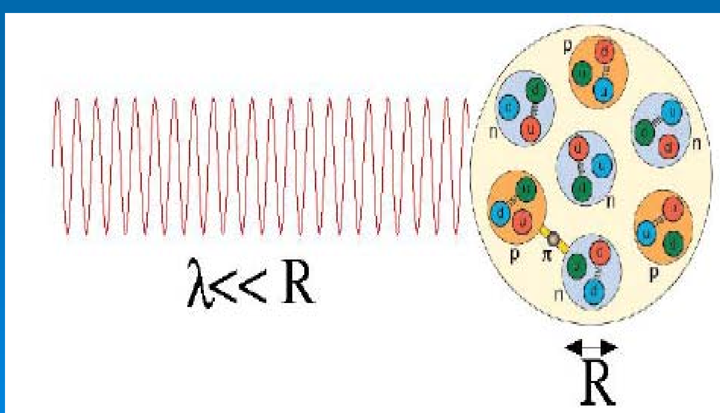
Answer: It depends on the energy scale!

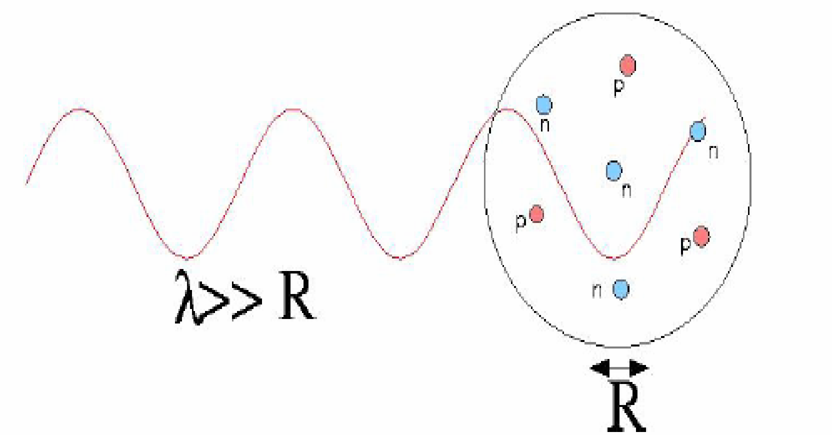






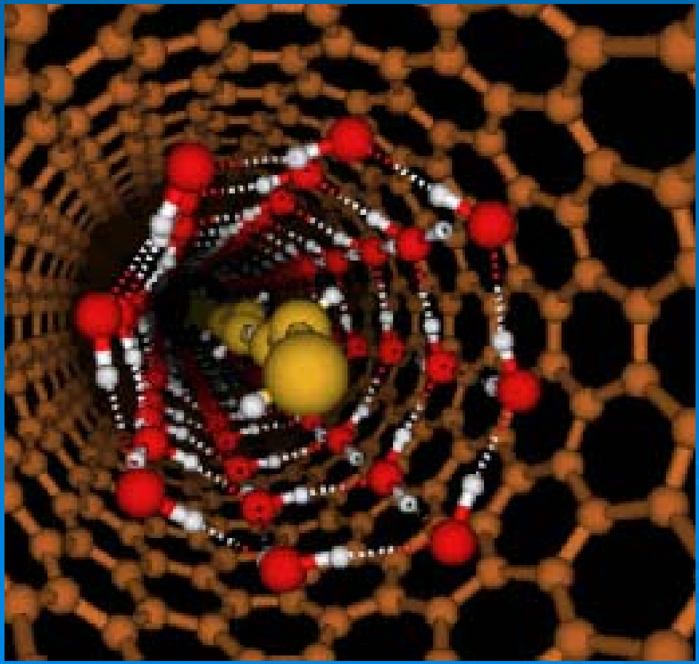
RHIC & CEBAF are our QCD machines.





- If system is probed at low energies, fine details not resolved
  - use low-energy variables for low-energy processes
  - short-distance structure can be replaced by something simpler without distorting low-energy observables

Another way to look at degrees of freedom



What makes sense to do:
-- Describe water via 1/r
   interactions between electrons?
-- Describe by incompressible
   fluid flow?

- Nano-water (1/r)
- Glass (fluid)

Kohn-Sham and Density Functional Theory

$$E[\rho] = \int \rho(\vec{r}) v(\vec{r}) d\vec{r} + F[\rho]$$

$$\delta\left\{E[\rho] - \mu\left[\int \rho(\vec{r}) d\vec{r} - N\right]\right\} = 0 \quad \Rightarrow \quad \mu = v(\vec{r}) + \frac{\delta F[\rho]}{\delta \rho}$$

The density that minimizes the ground-state energy satisfies the Euler equation

$$\Omega[\psi_1, \psi_2, \ldots, \psi_N] = \sum_{i=1}^{N} \int d\vec{r}\, \psi_i^*(\vec{r}) \left(-\frac{1}{2}\nabla^2\right) \psi_i(\vec{r})$$

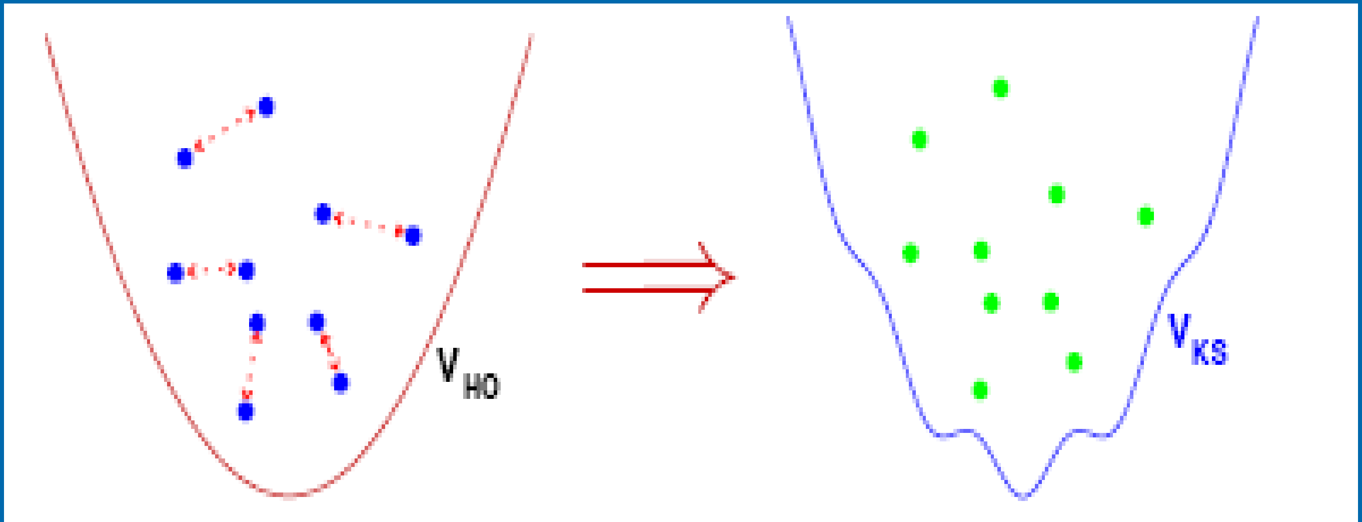
$$+ \int \lambda(\vec{r}) \left\{ \sum_{i=1}^{N} |\psi_i(\vec{r})|^2 - \rho(\vec{r}) \right\} d\vec{r} - \sum_{ij}^{N} \varepsilon_{ij} \int \psi_i^*(\vec{r}) \psi_j(\vec{r}) d\vec{r}$$

$$\frac{\delta \Omega}{\delta \psi_k^*(\vec{r}\,')} = 0 \quad \Rightarrow \quad \hat{h}_s \psi_k = \sum_{i=1}^{N} \varepsilon_{kl} \psi_l \quad \Rightarrow \quad \hat{h}_s \psi_k = \varepsilon_k \psi_k$$

$$\hat{h}_s = -\frac{1}{2}\nabla^2 + \lambda(\vec{r}) \quad \Rightarrow \quad \lambda(\vec{r}) = v(\vec{r}) + \frac{\delta F[\rho]}{\delta \rho}$$

Derivation in terms of single particle wave functions. Here the kinetic energy term is taken as exact

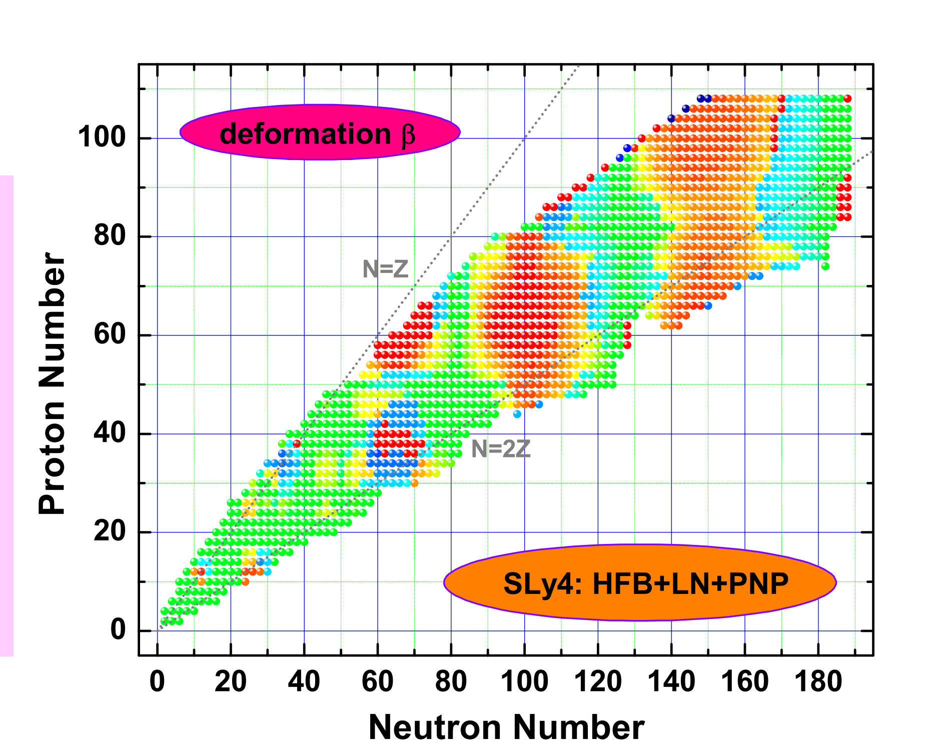
What is DFT accomplishing?



- Interacting potential replaced by non-interacting potential
- Orbitals are in a local potential (and there is no M*).
- Find V_{KS} from $\delta E/\delta\rho$ by solving the self-consistent equations

"Skyrme HF" is almost DFT, and is very close if M*=1
Challenge: Build DFT from 1) wave functions and densities from ab initio studies, and 2) from an EFT based formalism

Self-consistent mean field theory: Nuclear DFT



Recent developments:

- General nuclear energy density functional that allows proton-neutron couplings
- First fully self-consistent QRPA+HFB
- Development of formalism for exact particle number projection before variation (but problematic)
- Mass tables calculated

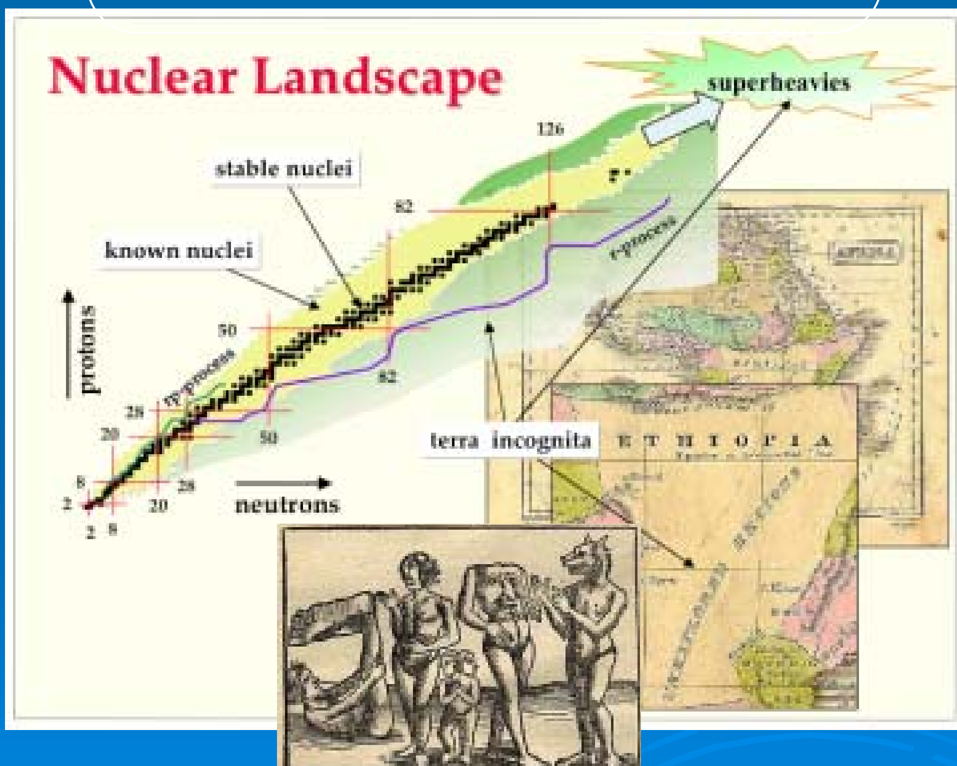
Nuclear DFT Challenges:

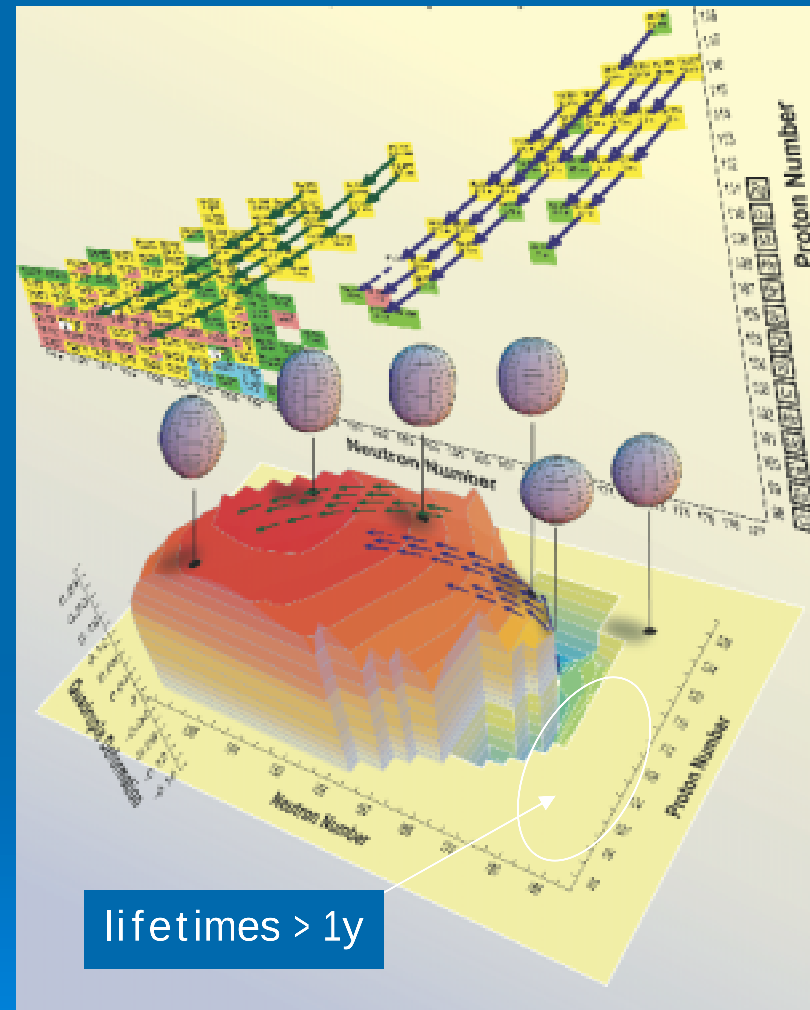
- Implement exact particle number projection (and others) before variation
- Improvement of the density dependence of the effective interaction
- Proper treatment of time-odd fields
- Inclusion of dynamical zero-point fluctuations
- Provide proper continuum basis for QRPA calculations

Stoitsov, Dobaczewski, Nazarewicz, Engel, Van Gai, Gorioly, Heenen, Duguet, Furnstahl, Bertsch ….

Challenge: Determine the limits of atoms and nuclei

Three frontiers, relating to the determination of the proton and neutron drip lines far beyond present knowledge, and to the synthesis of the heaviest elements

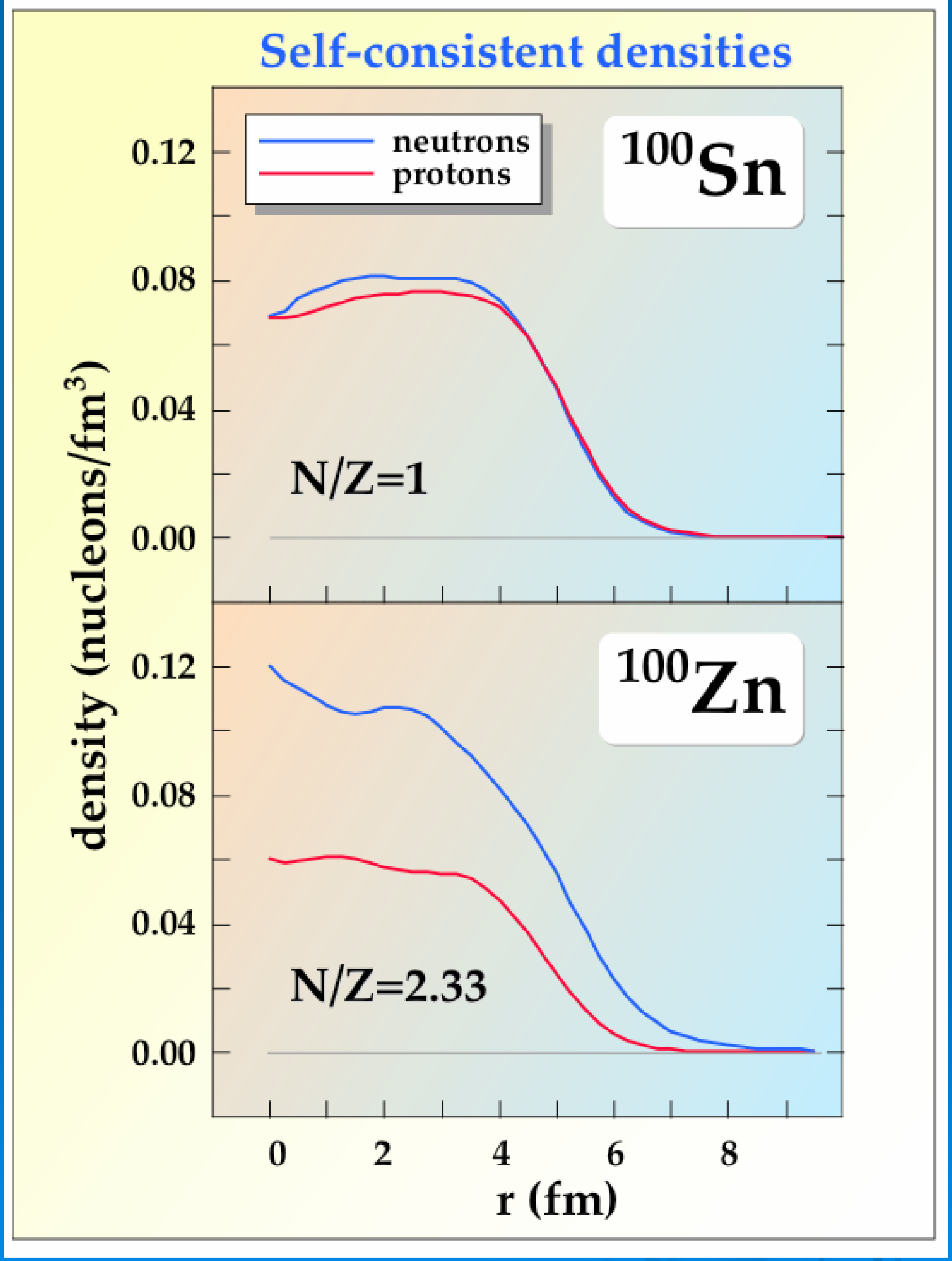


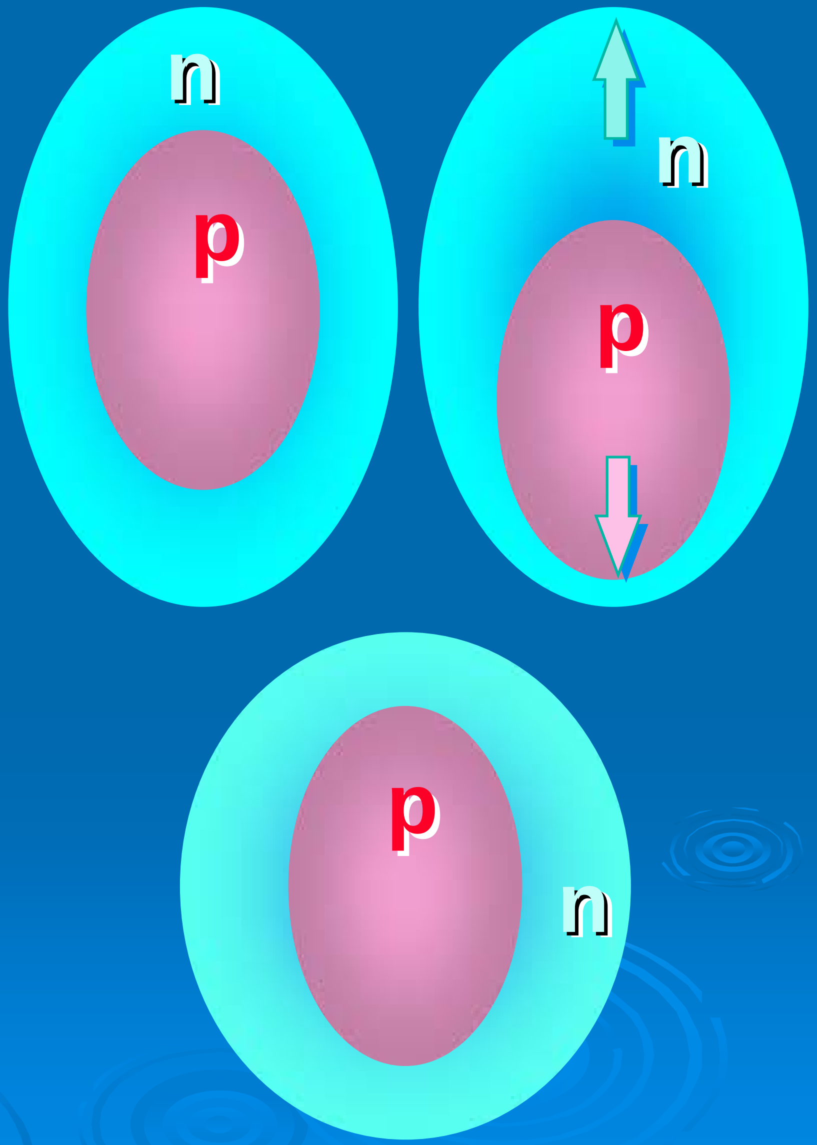


Do very long-lived superheavy nuclei exist?
What are their physical and chemical properties?

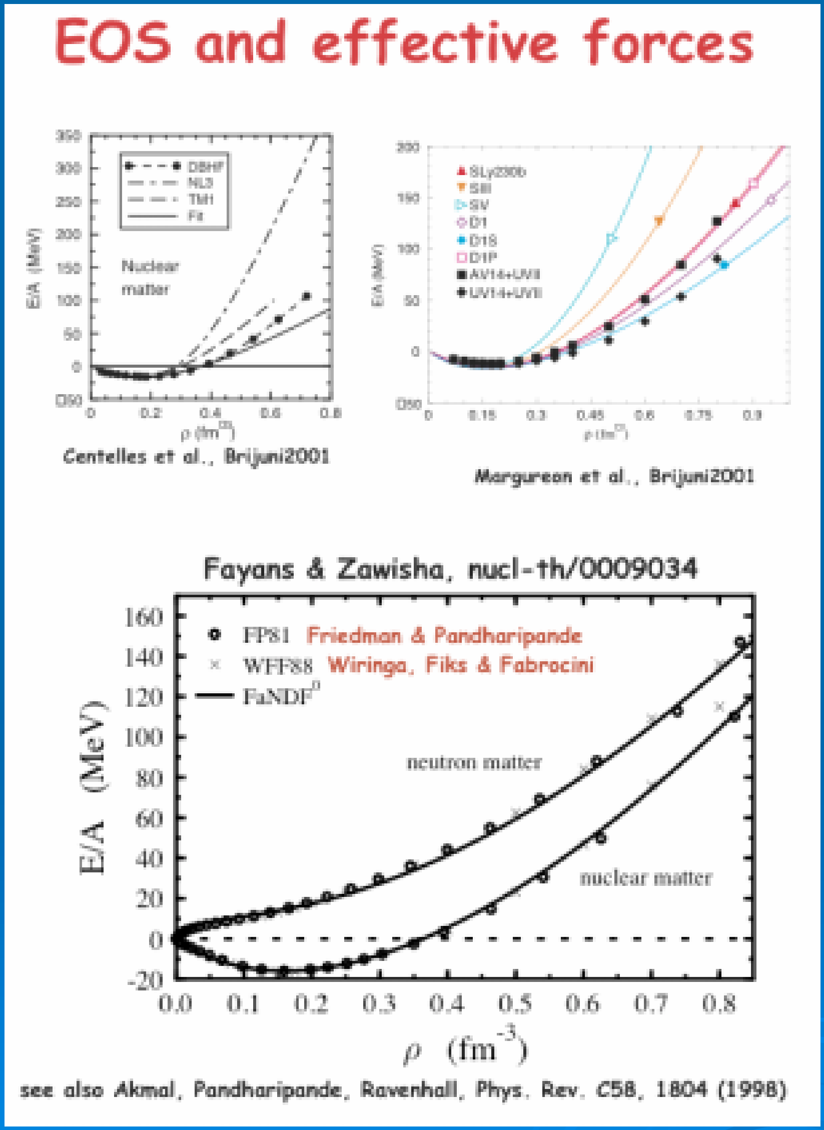
Shape coexistence and triaxiality in the superheavy nuclei
Cwiok, S.; Heenen, P.-H.; Nazarewicz, W.
***Nature*, v 433, n 7027, 17 Feb. 2005, p 705-9**

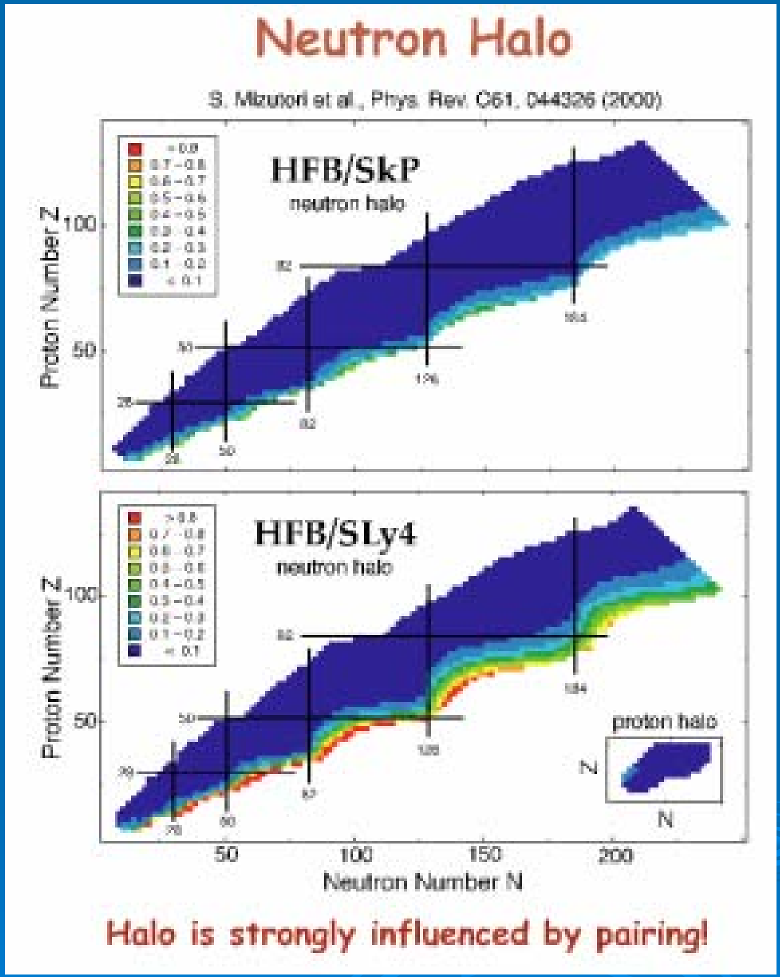
Skins and Skin Modes





Towards the Nuclear Energy Density Functional
(Equation of State)



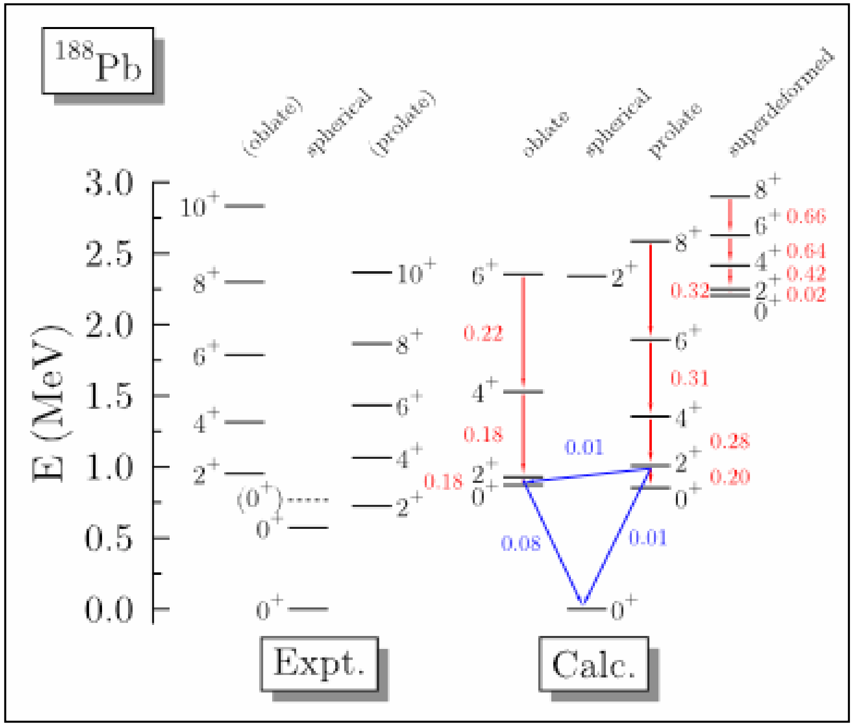


Challenges:
- density dependence of the symmetry energy
- neutron radii
- clustering at low densities

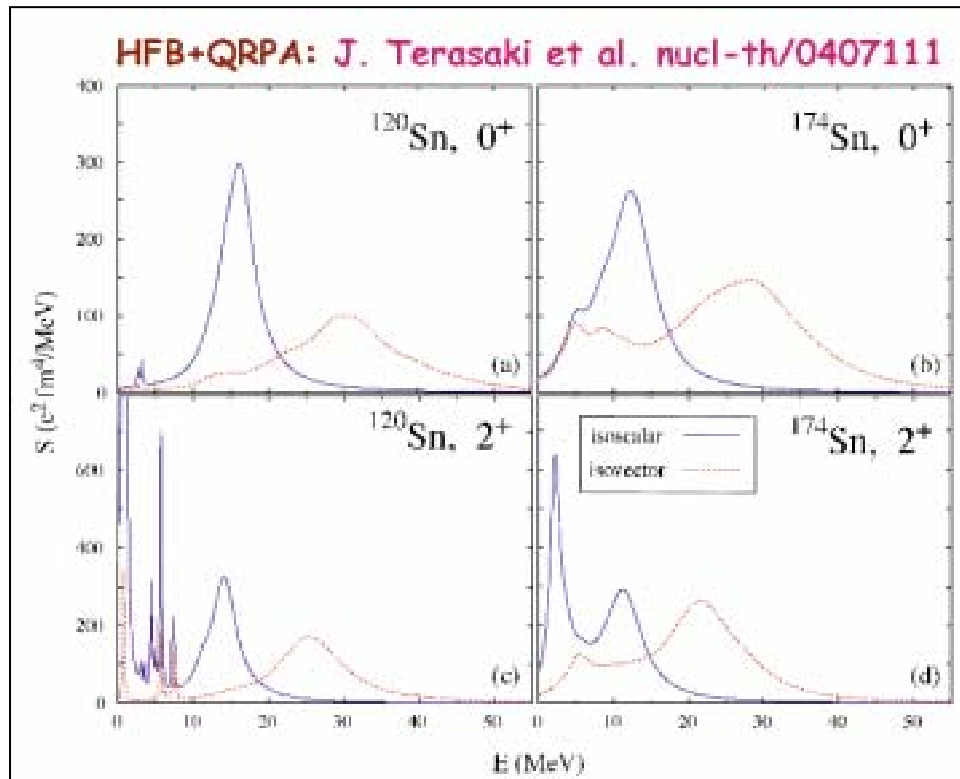
Beyond Mean Field

examples

M. Bender et al., PRC 69, 064303 (2004)



Shape coexistence



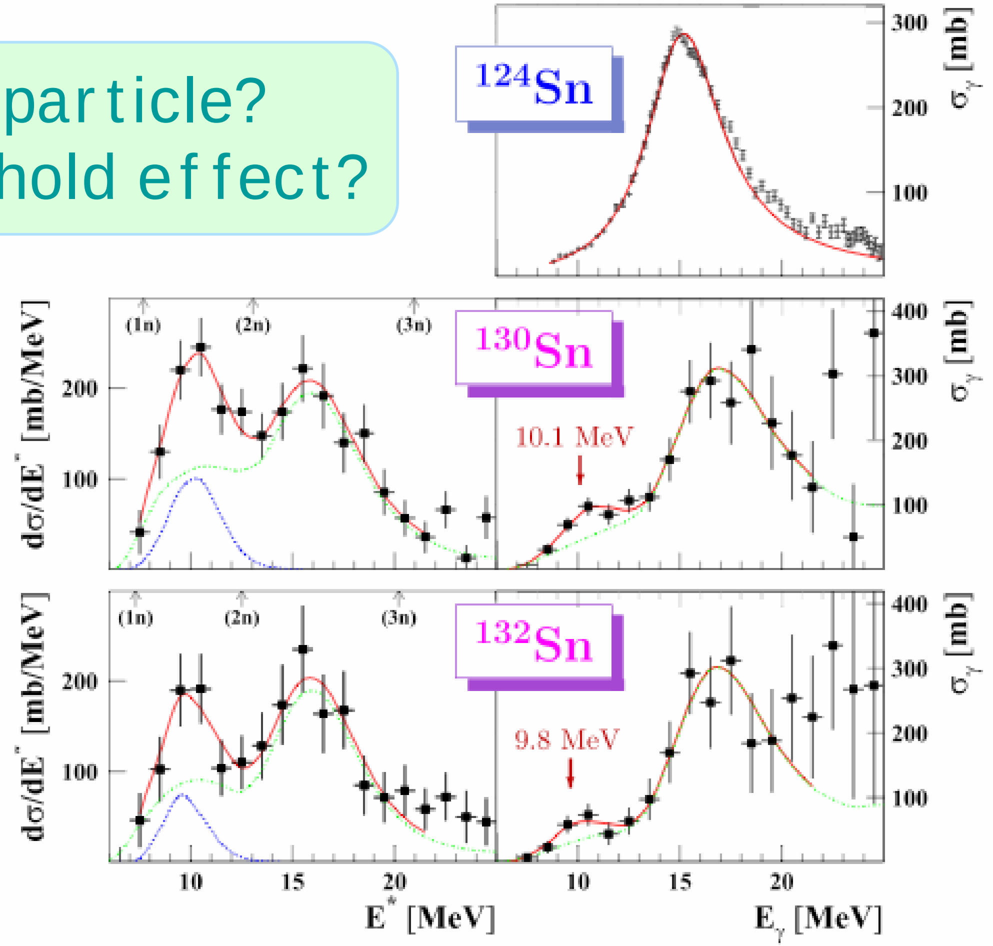
Soft modes in drip-line nuclei

PRL 95, 132501 (2005) PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2005

Evidence for Pygmy and Giant Dipole Resonances in ^{130}Sn and ^{132}Sn

P. Adrich,[1,4] A. Klimkiewicz,[1,4] M. Fallot,[1] K. Boretzky,[1] T. Aumann,[1] D. Cortina-Gil,[5] U. Datta Pramanik,[1] Th. W. Elze,[2] H. Emling,[1] H. Geissel,[1] M. Hellström,[1] K. L. Jones,[1] J. V. Kratz,[3] R. Kulessa,[4] Y. Leifels,[1] C. Nociforo,[3] R. Palit,[2] H. Simon,[1] G. Surówka,[4] K. Sümmerer,[1] and W. Walus[4]

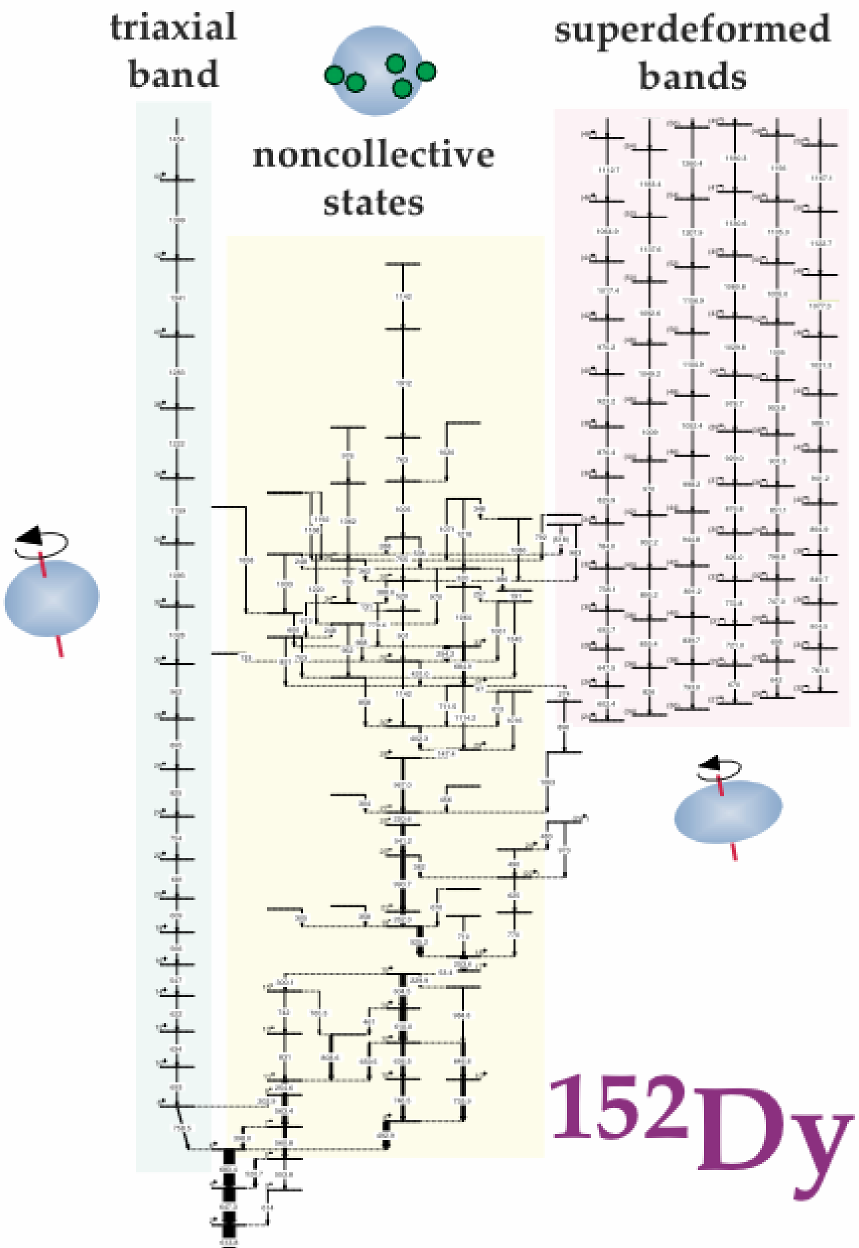
Collective or single-particle?
Skin effect? Threshold effect?

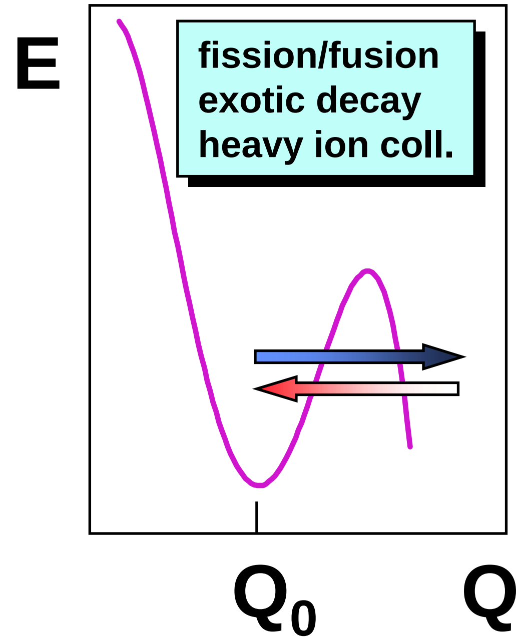


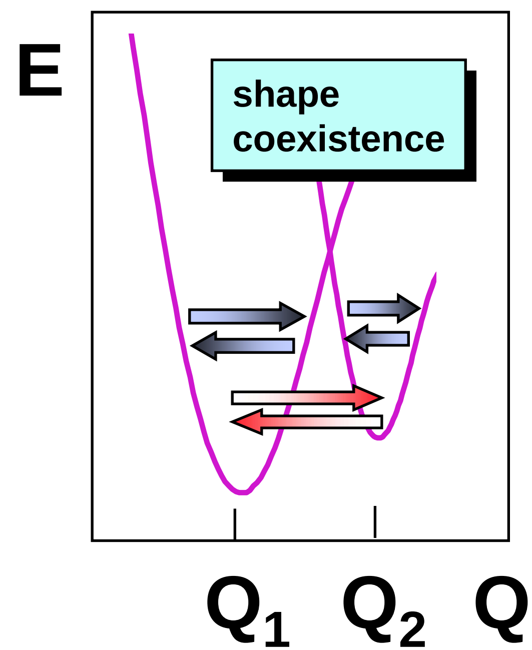
Energy differential electromagnetic dissociation cross section

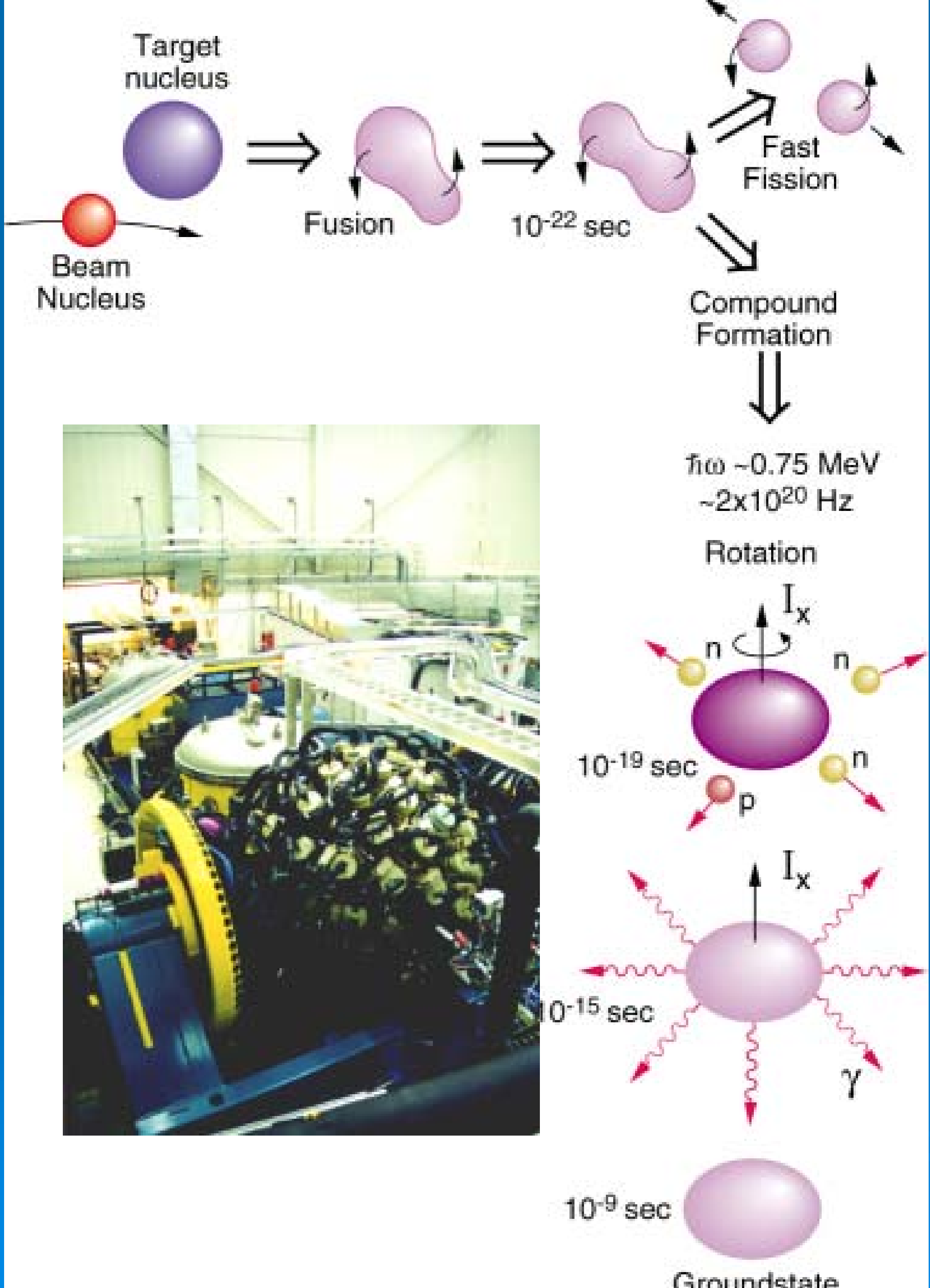
Deduced photo-neutron cross section.

Coexistence of collective and noncollective motion









Some nuclear properties relevant to reactions:

- **nuclear shape**
- **single-particle energies**
- **neutron-nucleus potential**
- **nuclear mass**
- **level densities**

- **One can measure level densities**
- **'Back-shifted Fermi Gas' model is often used to describe level densities, but is parameterized for each nucleus.**
- **Vast literature on improvements**
- **Necessary input to reaction cross section calculations:**
  - **-- 1p-1h, 2p-2h, np-nh, states**
  - **-- spin-level density**

A few words about nuclear reactions: level densities

$$Z(\beta) = \int e^{-\beta E} \rho(E) dE$$

almost impossible to solve, so use saddle-point approximation…

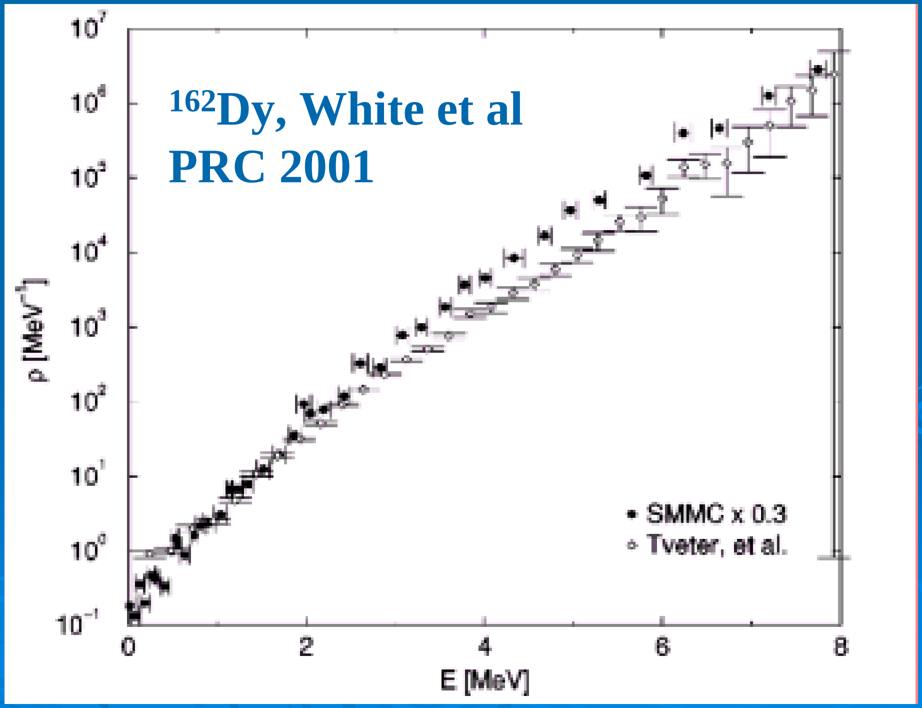
from SMMC calculation

$$\ln[Z(\beta)/Z(0)] = -\int_0^{\beta} d\beta' E(\beta')$$

$$S(E) = \beta E + \ln Z(\beta)$$

$$\rho(E) = \frac{\exp(S)}{\sqrt{2\pi\beta^{-2}C}}$$

$$\beta^{-2}C = -\frac{dE}{d\beta}$$



Thermal properties of finite nuclei: general considerations

- Remnants of phase transitions in finite systems:
  - ordered to disordered
  - paired – unpaired (~ 0.7-1.0 MeV)
  - deformed – spherical

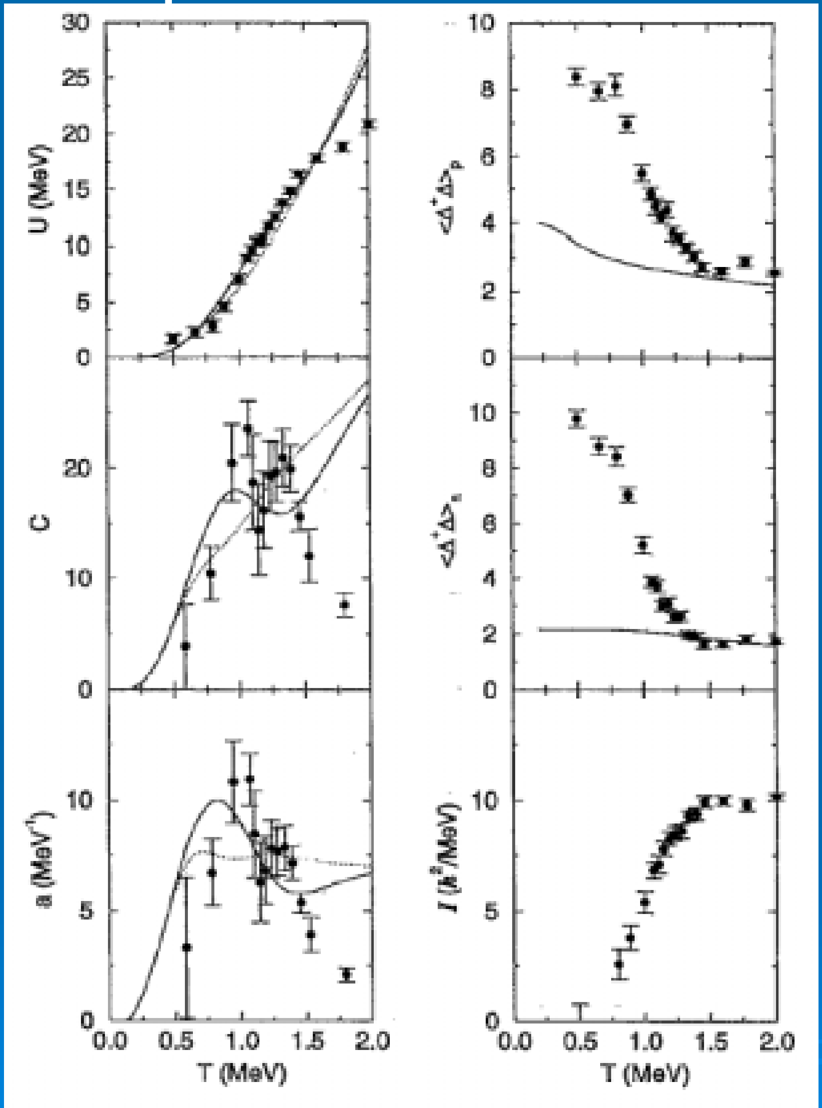
→How are pairing and deformation affected by temperature?

→How is rotational motion affected by temperature?

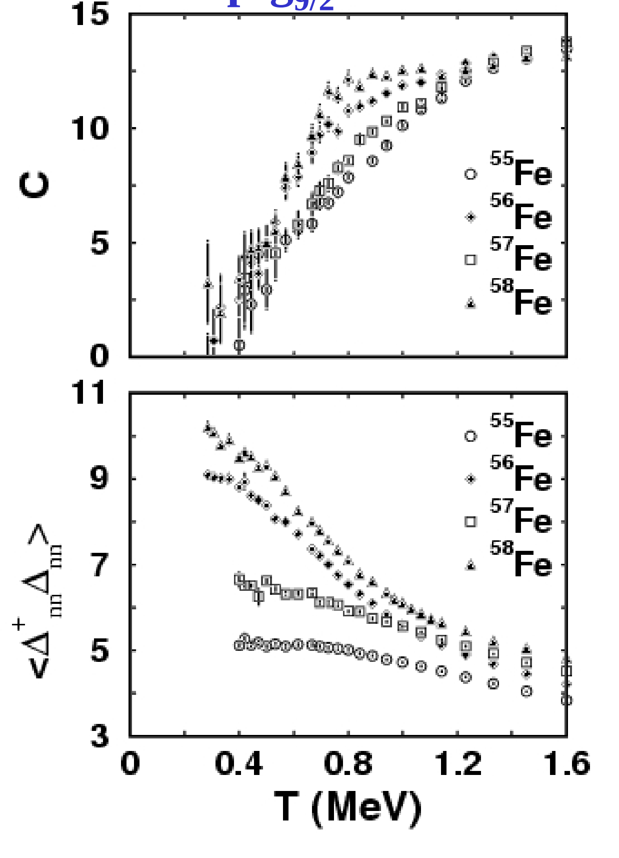
→ Connection to infinite matter?

SMMC studies of phase transitions

fp-shell ^{54}Fe



fp-$g_{9/2}$ shell



SMMC, pairing+quadrupole
(improved method to obtain C)

Liu & Alhassid, PRL 2000

SMMC: Realistic Hamiltonian; extrapolations.

Dean, Koonin, Langanke, Radha, Alhassid, PRL77, 1444 (1995)

PP+QQ, Ormand, 1998; Langanke, 1998

Pairing transitions in finite Fermi systems

- What are the thermodynamic properties of a finite many-body system?
- Can we characterize thermal transitions within finite systems?
- What is the role of the interaction in affecting transitions?

Microcanonical ensemble:

$\Omega(E)$ Density of states (microcanonical partition function)

$$F(E) = -T\ln\{\Omega(E)\exp(-\beta E)\}$$

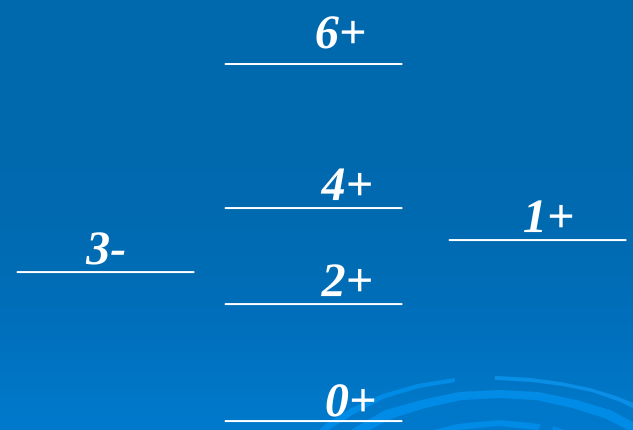
Free energy at a given E.

Canonical Ensemble:

$$Z(\beta) = \hat{\mathrm{T}}\mathrm{r}\left\{\exp\left(-\beta\hat{\mathrm{H}}\right)\right\} = \sum_E \Omega(E)\exp(-\beta E)$$

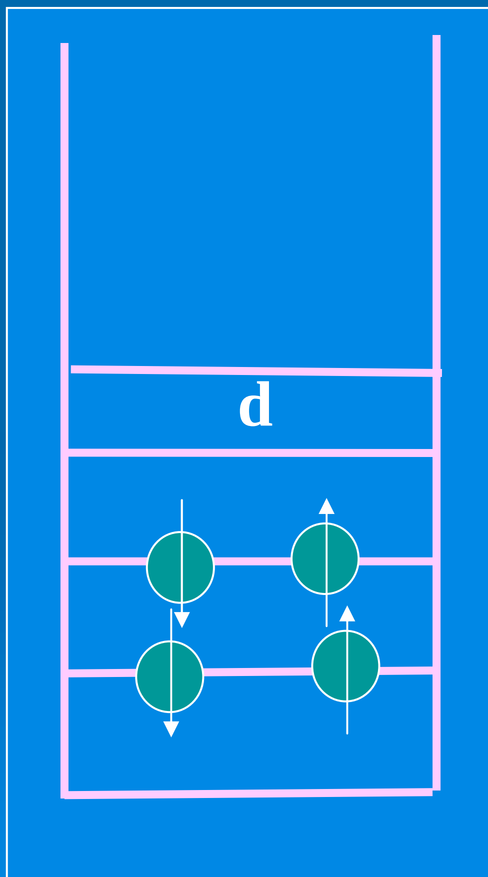
Analytic continuation of β:

$$Z(B);\ B = \beta + i\tau$$



Low-lying part of a typical nuclear spectrum

A very simple pairing problem with many physical applications



$$H = \sum_i \varepsilon_i a_i^+ a_i - G \sum_{ij} a_i^+ a_{\bar{i}}^+ a_{\bar{j}} a_j$$

$$H = d \sum_i i N_i - G \sum_{ij} S_i^+ S_j^-$$

d/G = 0.5 (normal pairing)
d/G = 2.0 (weak pairing)

Simple Theoretical Considerations

Microcanonical density of states

$$N(E,\beta,L) \equiv \frac{L}{Z(\beta)} w(E)\exp(-\beta E) \qquad A(E,\beta,L) = -\ln N(E,\beta,L)$$

Partition function

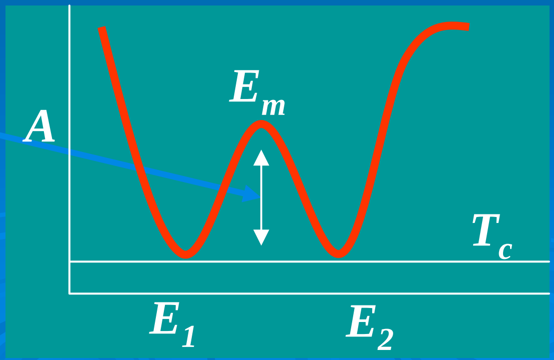
Lee and Kosterlitz, PRL65, 137 (1990) showed that if a system exhibits a transformation in phase at a temp T_c, then

$$A(E_1,\beta) = A(E_2,\beta)$$

$$\Delta F = A(E_m,\beta) - A(E_1,\beta)$$

$$F \propto A$$

if Z varies slowly near T_c



Follow ΔF as system size increases:

- **Increasing: 1st order**
- **constant: 2nd order**
- **Decreasing: Ordered to disordered**

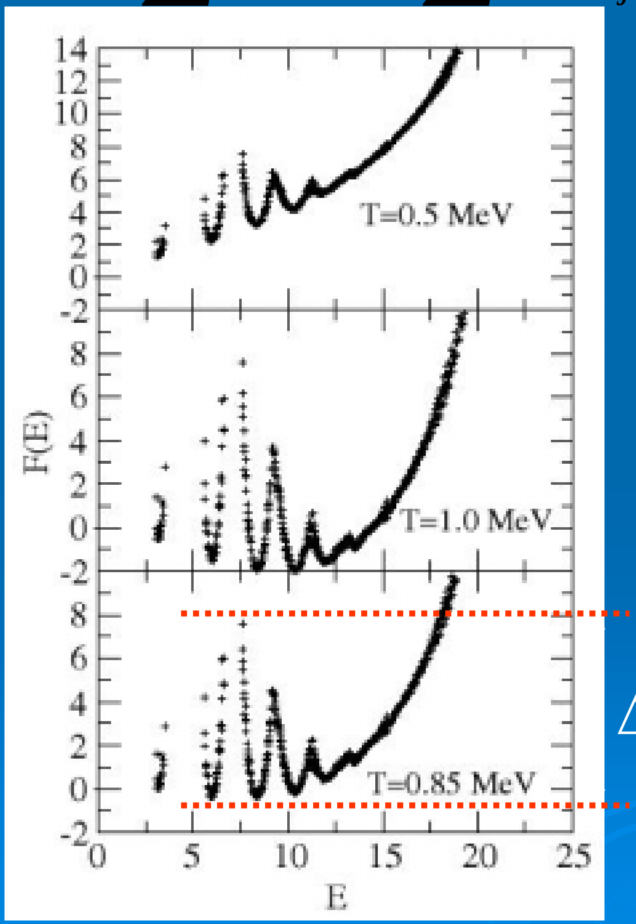
Investigation of a pure pairing model

$$H = \sum_i \varepsilon_i a_i^+ a_i - G \sum_{ij} a_i^+ a_{\bar{i}}^+ a_{\bar{j}} a_j$$

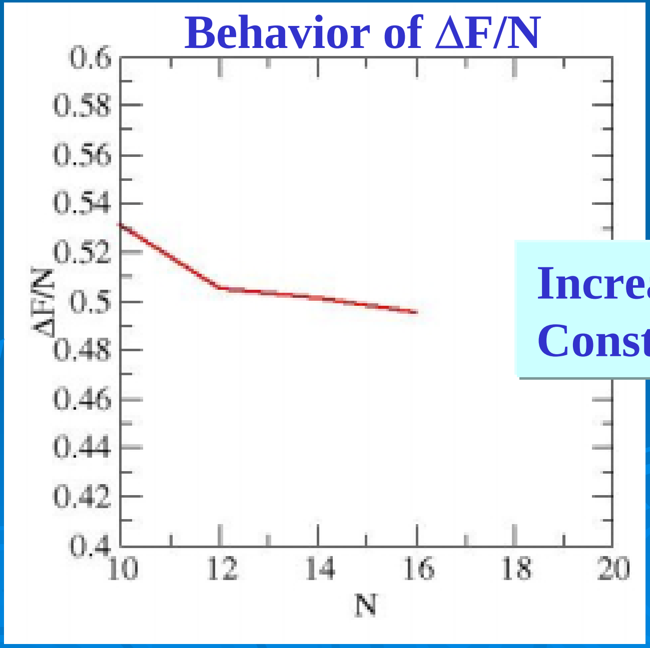
$$H = d \sum iN_i - G \sum S_i^+ S_j^-$$

- Essentially the Richardson model
- Diagonalize and find all states

d/G = 0.5 (normal pairing)
d/G = 2.0 (weak pairing)



ΔF



Increasing: 1st order
Constant: 2nd order

Belic, Dean, Hjorth-Jensen, NPA731, 381 (2004)
Dean and Hjorth-Jensen, Rev. Mod. Phys. 75, 607 (2003)

Analytic continuation of the partition function

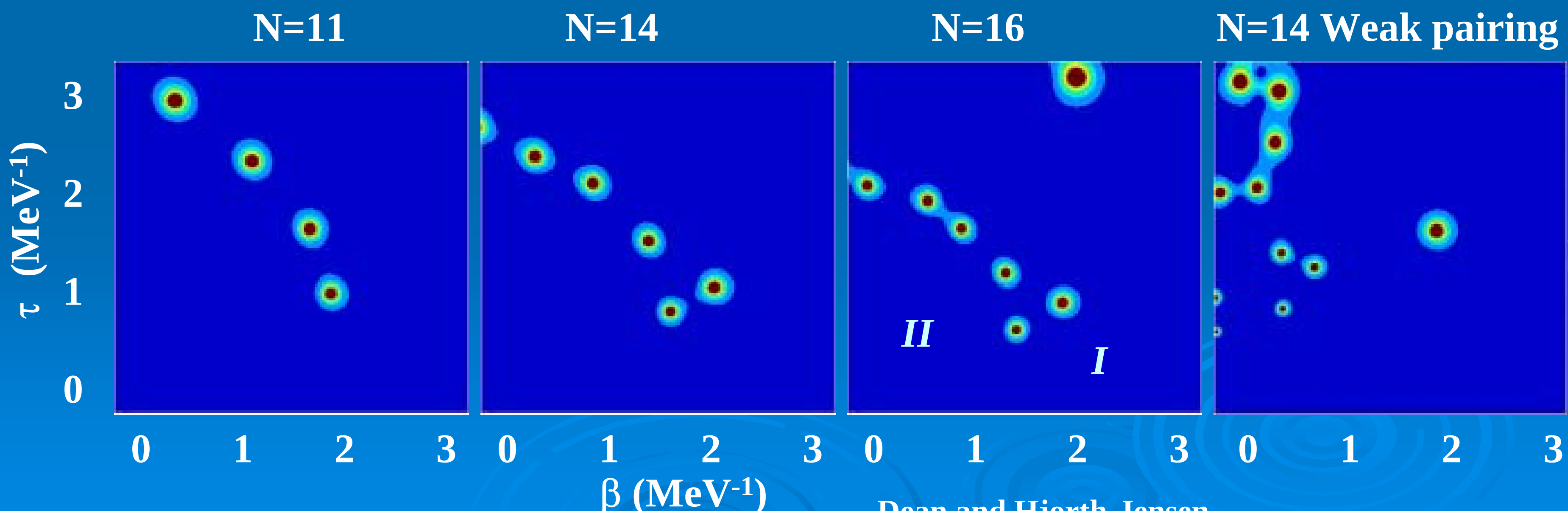
See Borrmann et al., PRL84, 3511 (2000)
(non-interacting bosonic systems)
Grossmann & Rosenhauer, Ziet. Phys. 207, 138 (1967)
(infinite systems)

$$Z(B)=\sum_E \Omega(E)\exp(-BE)$$

- Density of zeros (or poles in the specific heat)
- characterized by
  - γ = angle of approach to real axis
  - α = slope (sort of) of line at small τ
  - τ_1= closest zero (finite size effect)

$\alpha=\gamma=0$ First order

$0<\alpha<1$ any γ Second order



Dean and Hjorth-Jensen,
Rev. Mod. Phys. 75, 607 (2003)

Interpretation of the analytic continuation

$$Z(B) = \hat{\mathrm{T}}\mathrm{r}\left\{\exp\left(-\beta\hat{H} - i\tau\hat{H}\right)\right\}$$

$$= \sum_{\alpha}\left\langle\alpha\right|\exp\left(-\frac{\beta}{2}\hat{H}\right)\exp\left(-i\tau\hat{H}\right)\exp\left(-\frac{\beta}{2}\hat{H}\right)\left|\alpha\right\rangle$$

$$= \left\langle\Psi(t=0)\middle|\Psi(t=\tau)\right\rangle$$

= time evolved overlap.
Z(B)=0 represents a boundary.

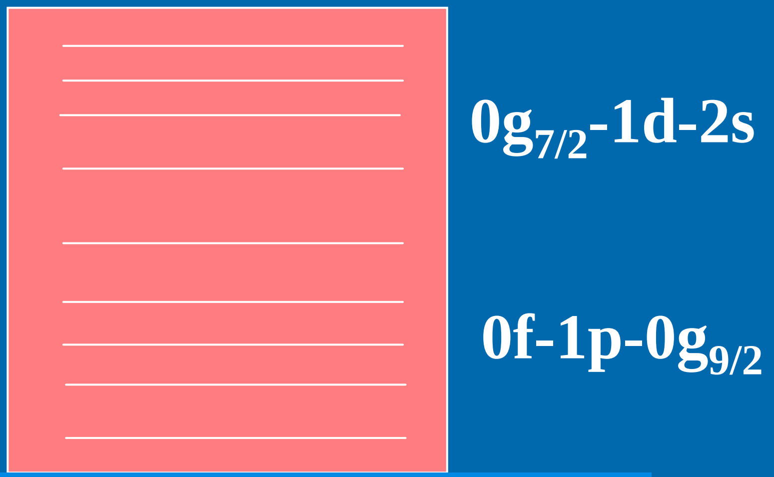
Thermal ensemble

Time evolution of thermal ensemble

- **Zeros of Z are boundary points that indicate when the system looses memory of its initial state.**
- **Zeros closest to real axis contribute the most to the specific heat of the system.**

Thermal effects on pairing *and deformation* in nuclear systems

Pairing+Quadrupole Hamiltonian:
solve using Auxiliary Field
Monte Carlo techniques.



fp-gds model space (^{40}Ca is the core)

10^{20} many-body basis states

^{68}Ni → Spherical ground state; weak N=40 shell closure
^{70}Zn → stronger proton pairing correlations;
some quadrupole collectivity; erosion of N=40 shell gap
^{72}Ge → shape coexistence phenomena; static proton and
neutron pairing
^{80}Zr → very deformed; large N=40 shell effects, weakened pairing

Langanke, Dean, Nazarewicz, Nucl. Phys. A (2005)
Dean, Nazarewicz, Langanke (in prep, 2006)

Simple AFMC

Single-particle energy

two-body interaction

$$\hat{H} = \varepsilon\hat{\Omega} + \frac{V}{2}\hat{\Omega}^2$$

We want:

$$Z = \mathrm{Tr}\left[\exp\left(-\beta\hat{H}\right)\right] \quad \rightarrow \quad \left\langle \hat{H} \right\rangle = \frac{\mathrm{Tr}\left[\exp\left(-\beta\hat{H}\right)\hat{H}\right]}{Z}$$

use the Hubbard-Stratonovich transformation

$$\exp\left(-\beta\hat{H}\right) = \sqrt{\frac{\beta|V|}{2\pi}}\int_{-\infty}^{\infty} d\sigma \exp\left(-\beta|V|\sigma^2/2\right)\exp\left(-\beta\hat{h}\right)$$

$$\hat{h} = \varepsilon\hat{\Omega} + sV\sigma\hat{\Omega}$$

$$s = 1 \quad for \quad V < 0$$
$$s = i \quad for \quad V > 0$$

Koonin, Dean, Langanke, Phys. Rep. 278, 2 (1997)

Auxiliary Field Monte Carlo

In general:

Trotter approx **HS**

$$Z = \mathrm{Tr}\left[\exp(-\beta\hat{H})\right] \rightarrow \mathrm{Tr}\left[\exp\left(-\Delta\beta\hat{H}\right)\right]^{N_t} \rightarrow$$

$$\int D[\sigma]G(\sigma)\mathrm{Tr}\left\{\prod_{n=1}^{N_t}\exp\left[(-\Delta\beta\hat{h}(\sigma_n))\right]\right\} = \int D[\sigma]W(\sigma)\Phi(\sigma)$$

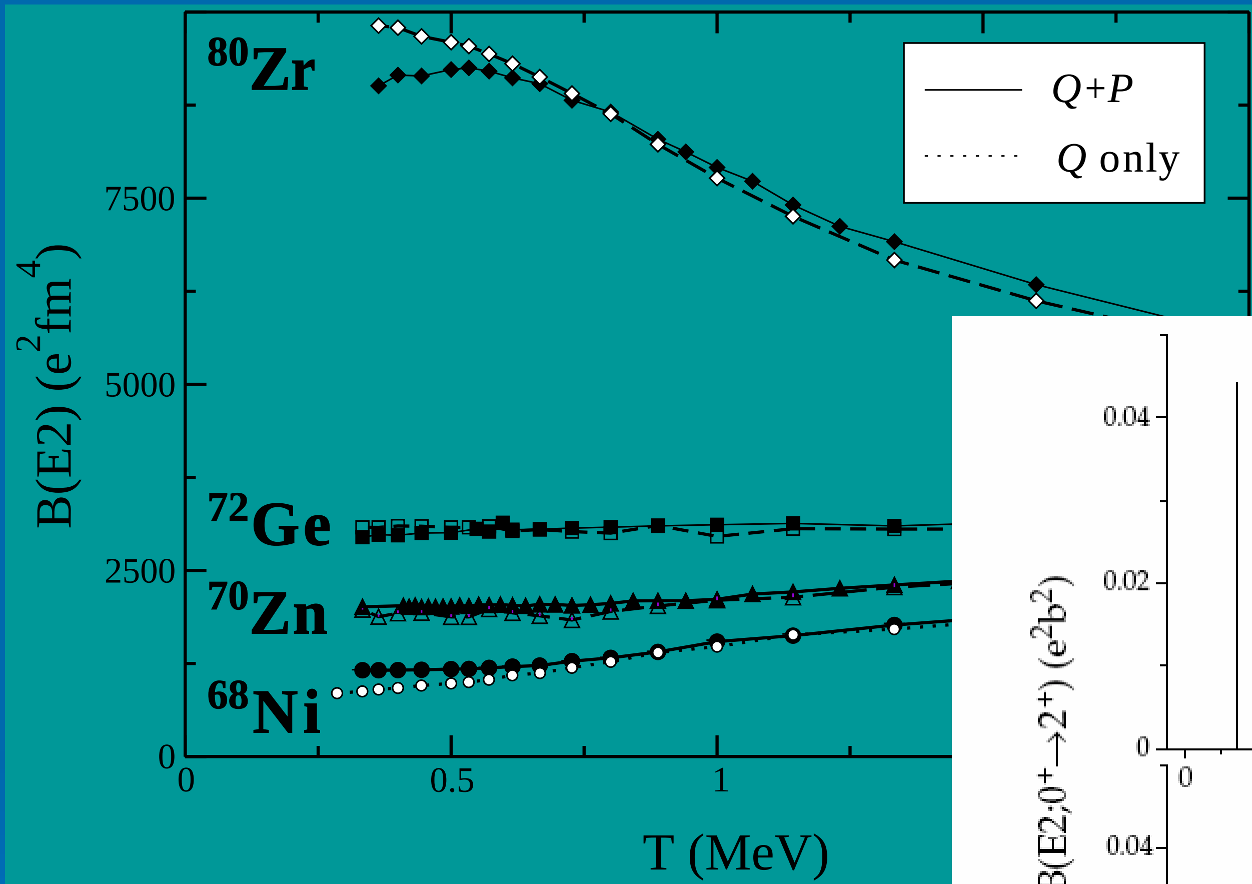
$$W(\sigma) = G(\sigma)\left|\mathrm{Tr}[\ ]\right| \qquad \Phi(\sigma) = \frac{\mathrm{Tr}[\ ]}{\left|\mathrm{Tr}[\ ]\right|}$$

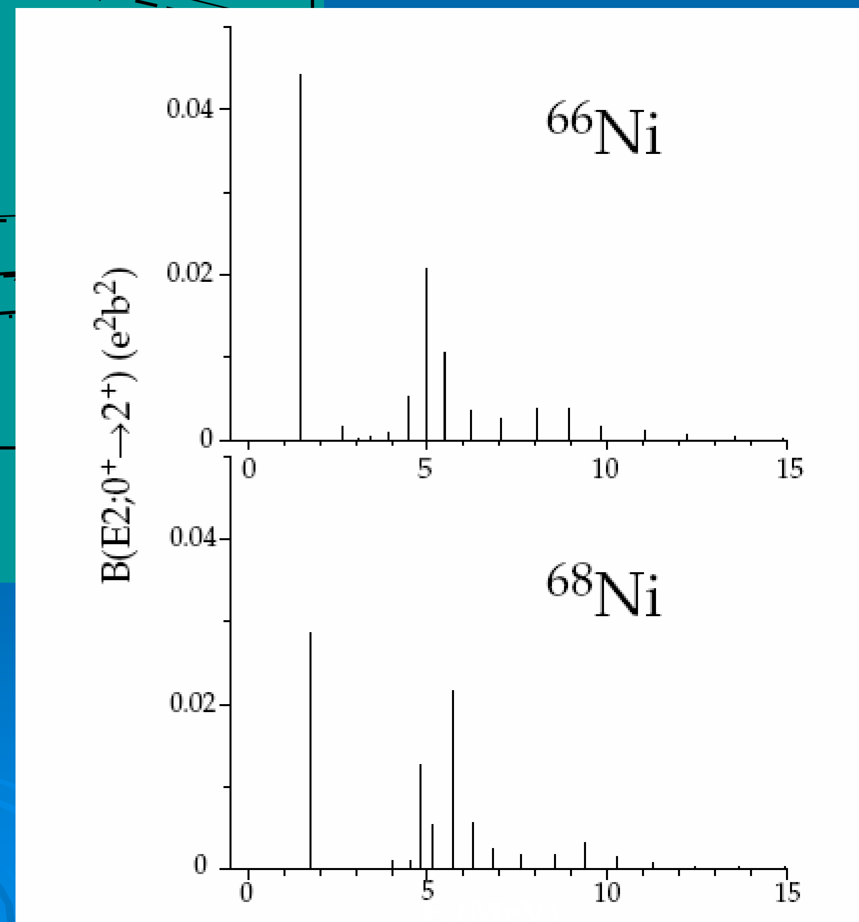
Number Projection (Canonical):

$$\mathrm{Tr}\left[\hat{\Omega}\right] \equiv \mathrm{Tr}_N\left[\hat{\Omega}\right] = \sum_i \left\langle i\left|\hat{P}_N\hat{\Omega}\right|i\right\rangle$$

$$\hat{P}_N = \delta\left(\hat{N} - N\right) = \int_0^{2\pi}\frac{d\varphi}{2\pi}\exp\left\{i\varphi\left(\hat{N} - N\right)\right\}$$

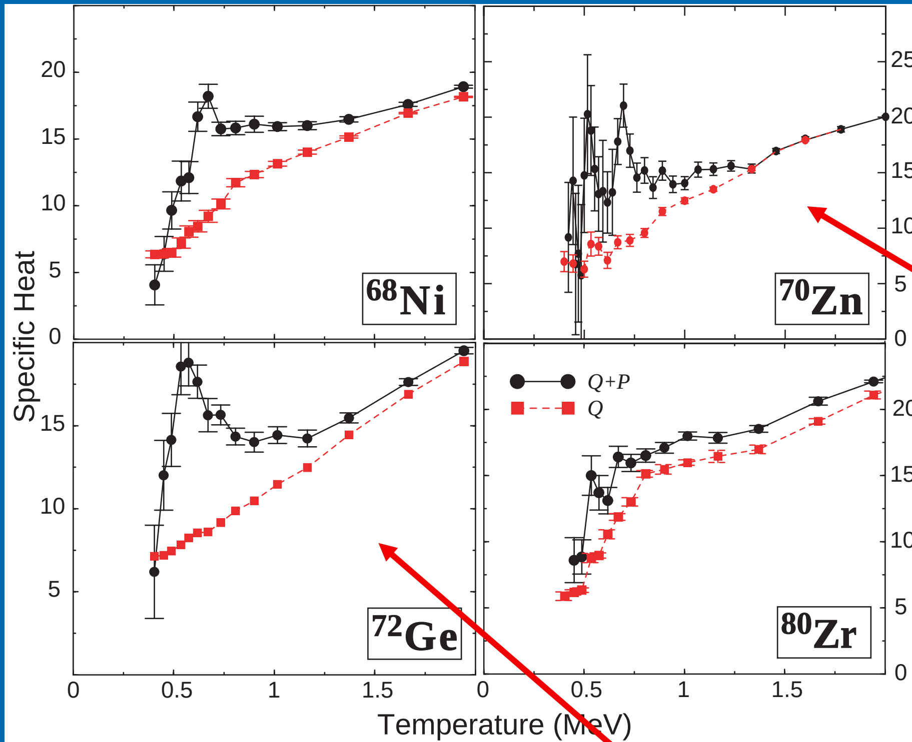
Total B(E2) as a function of temperature

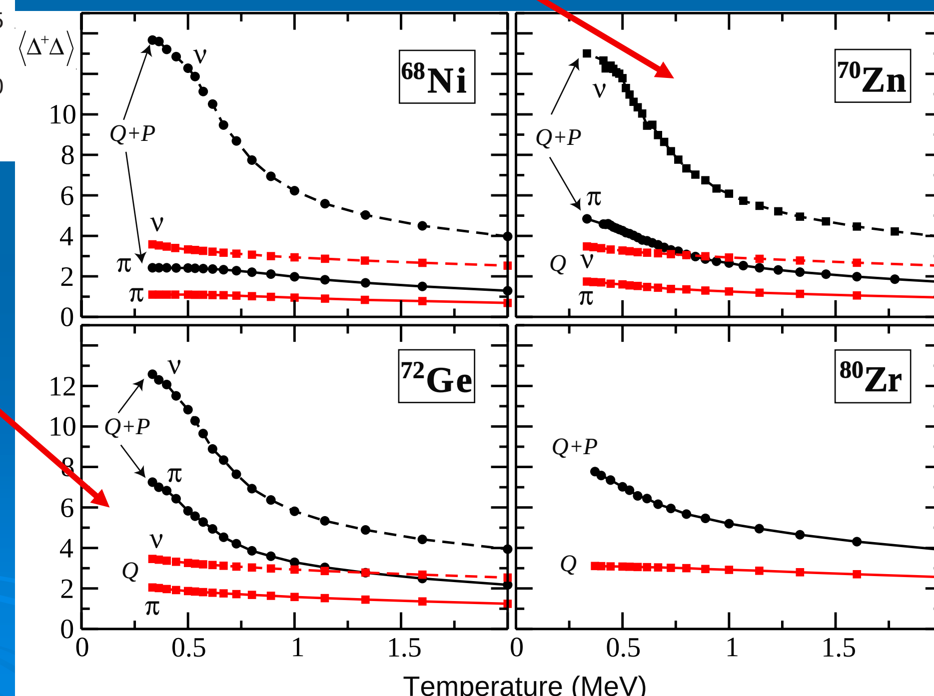




Langanke, Terasaki, Nowacki,
Dean, Nazarewicz, PRC61, 44314 (2003)

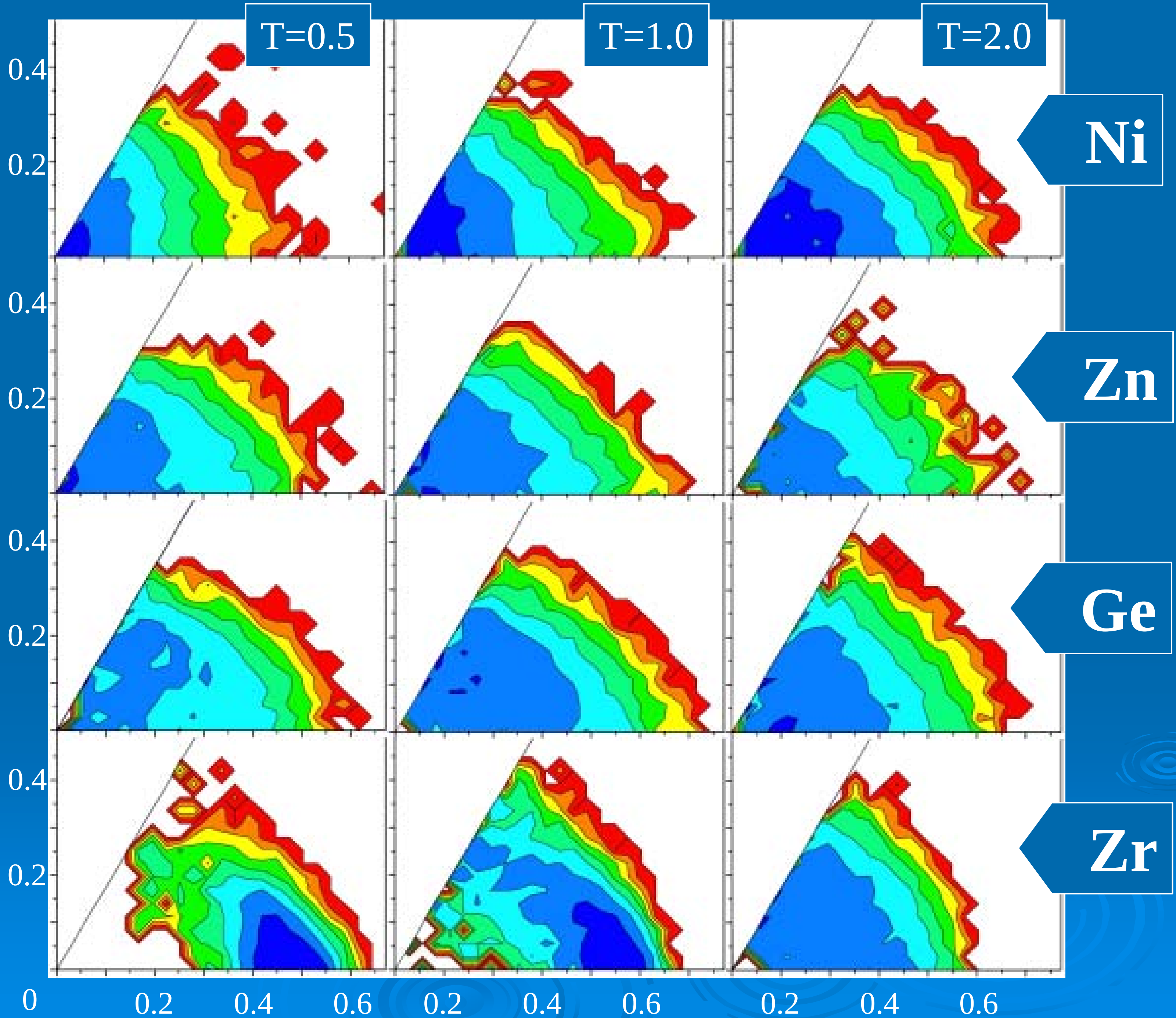
Pairing, deformation, and the specific heat



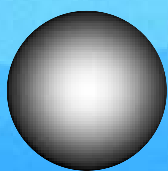


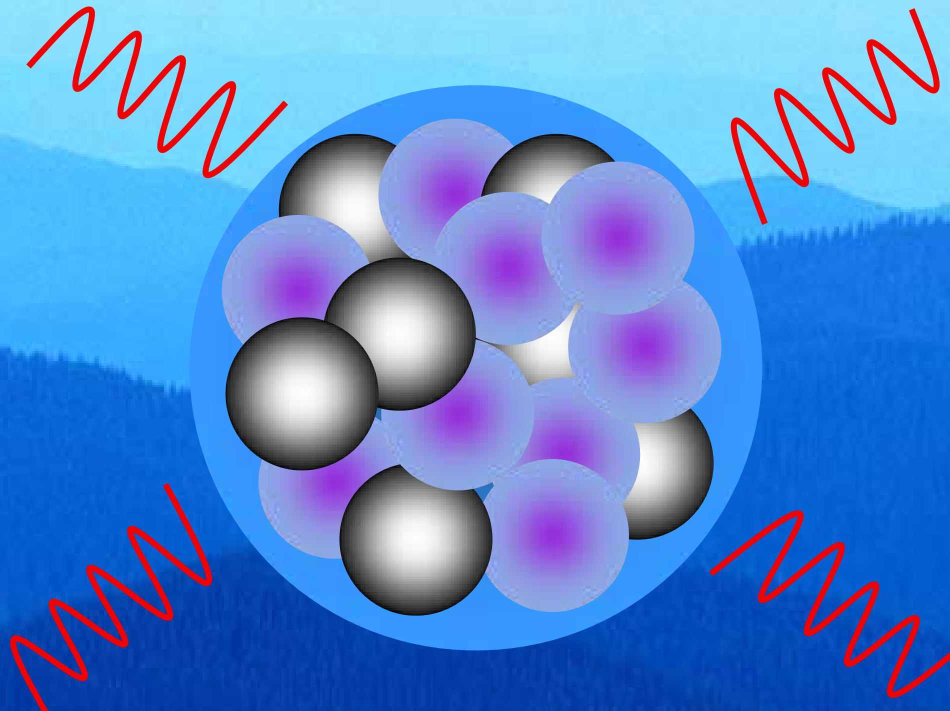
$$E(\beta) = \frac{Tr\left[\exp(-\beta H)H\right]}{Tr\left[\exp(-\beta H)\right]}$$

$$C_v = -\beta^2 \frac{dE}{d\beta}$$


T=0.5
T=1.0
T=2.0
Ni
Zn
Ge
Zr
0.4
0.2
0.4
0.2
0.4
0.2
0.4
0.2
0
0.2
0.4
0.6
0.2
0.4
0.6
0.2
0.4
0.6

Simple nuclear collision

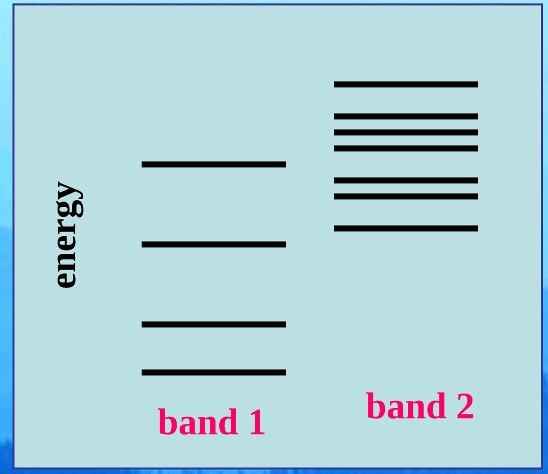




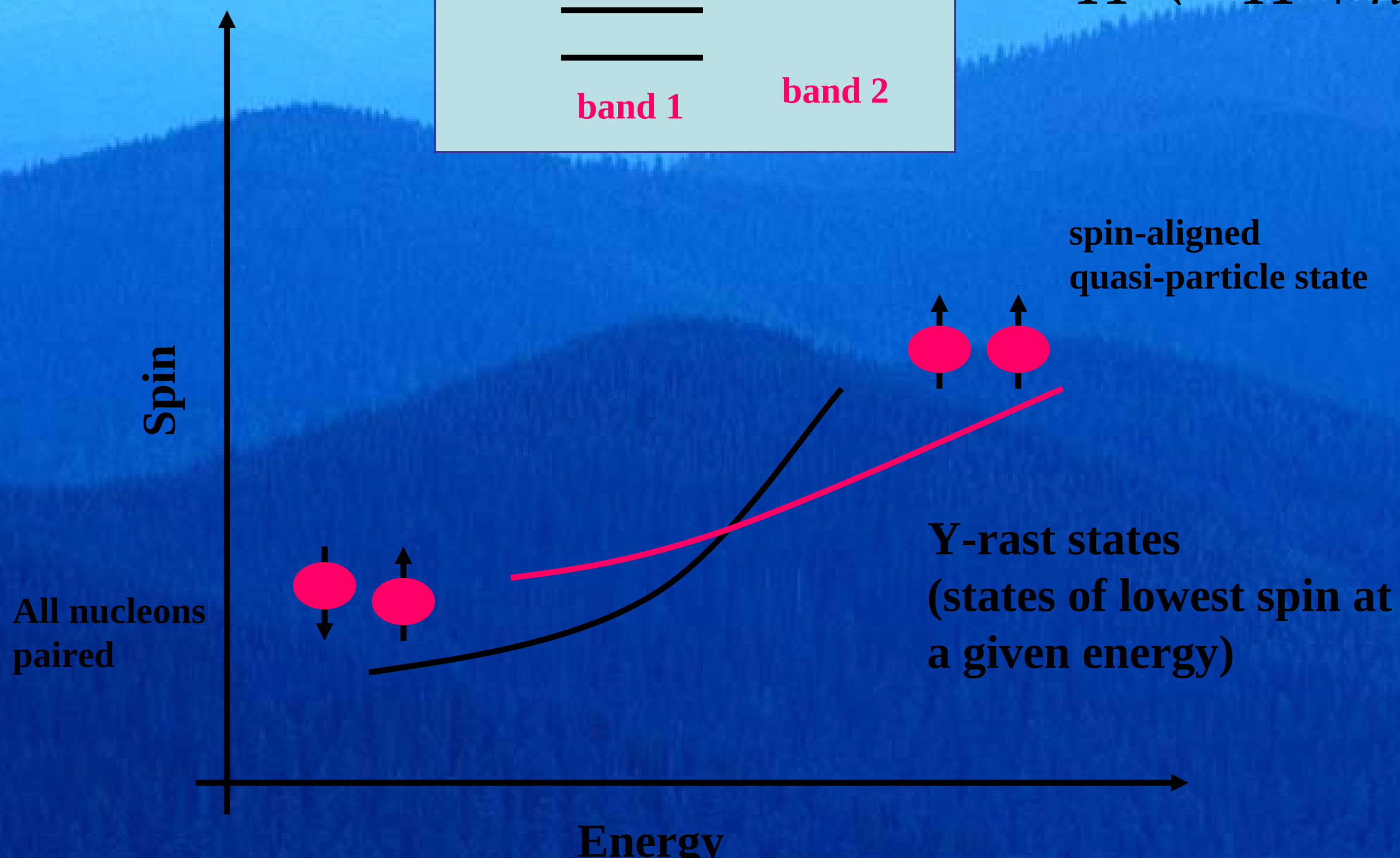
$$H' = H + \hbar\omega J_z$$

Nucleus spins down by emitting gammas
- Low spins: reduction in pairing → first quasi aligned band
- higher spins: super deformed bands

What happens to pairing in a (warm) rotating nucleus?

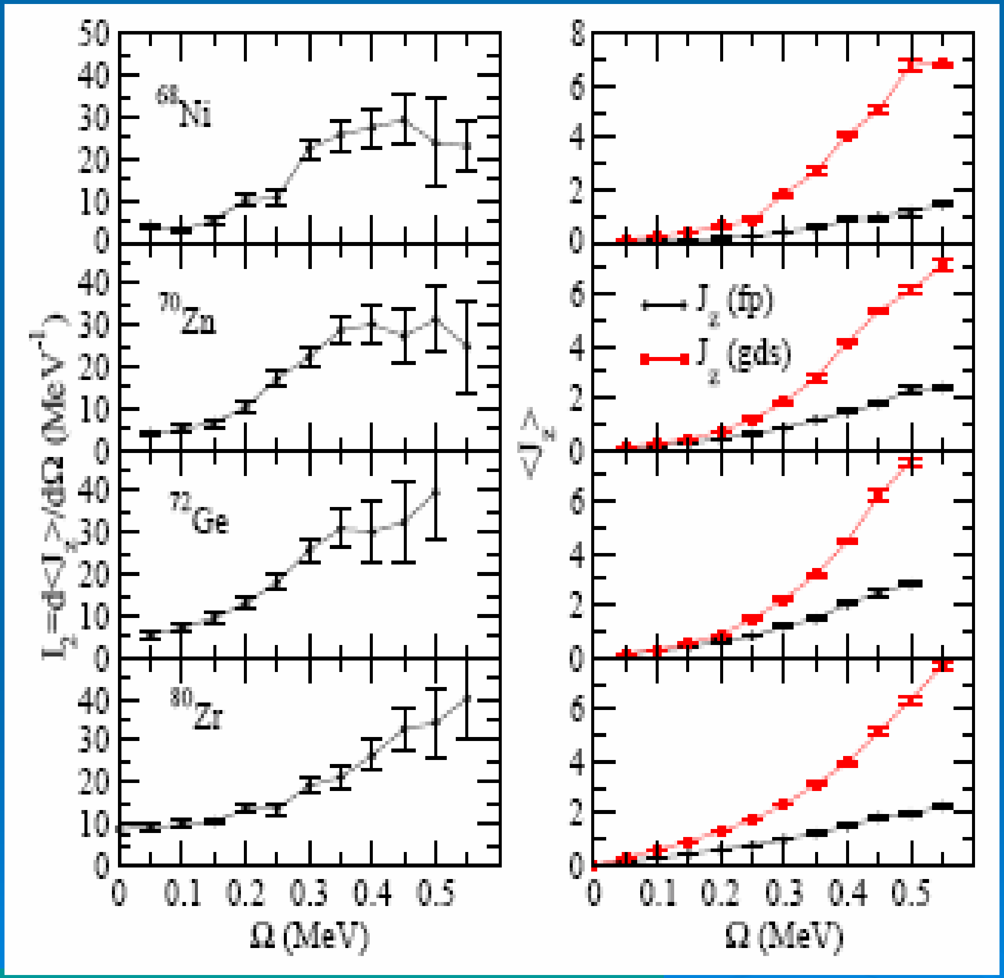


$$H \leftarrow H + \hbar\omega J_z$$



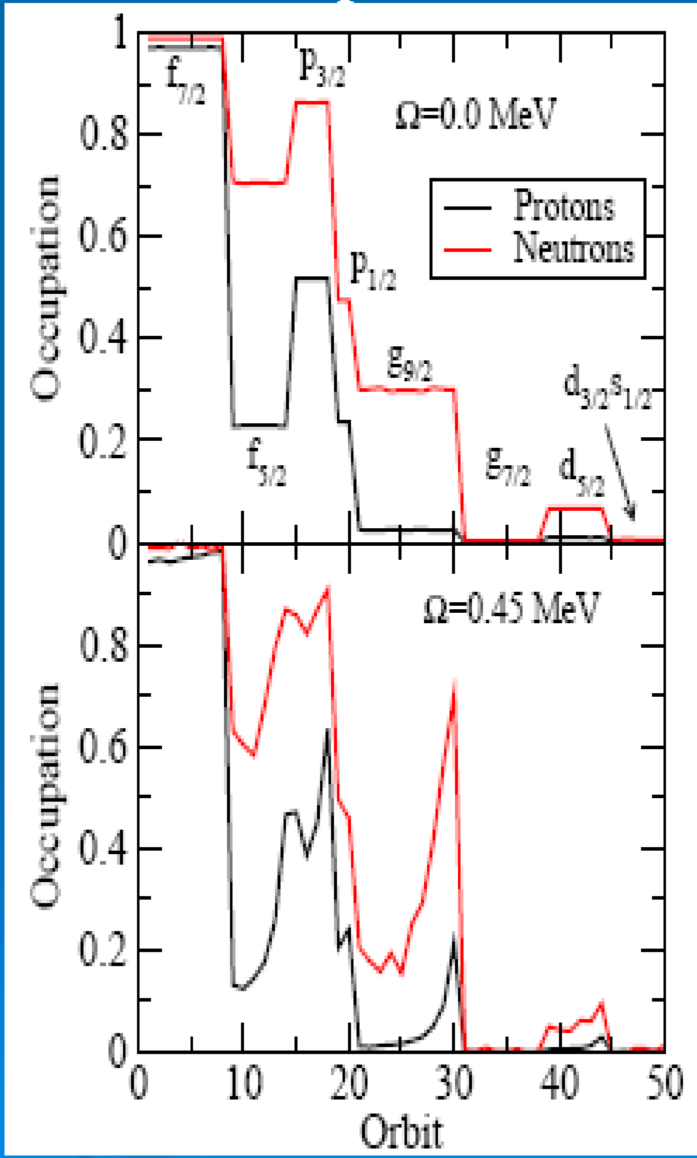
Rotational properties of the N=40 systems

$$H' = H + \omega J_z$$

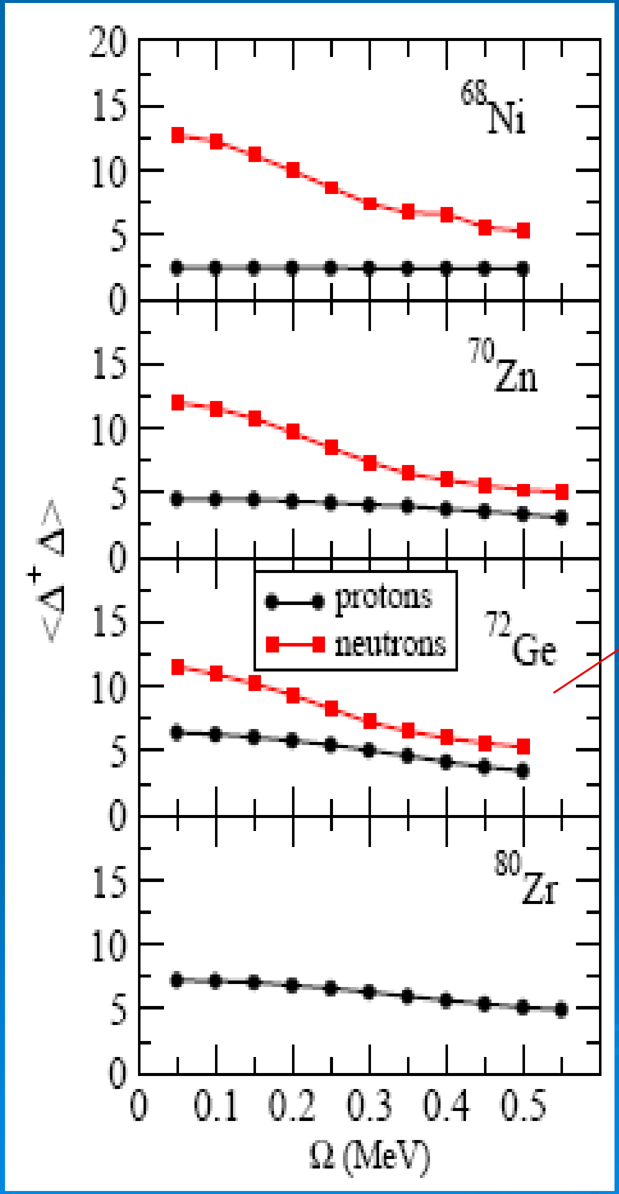


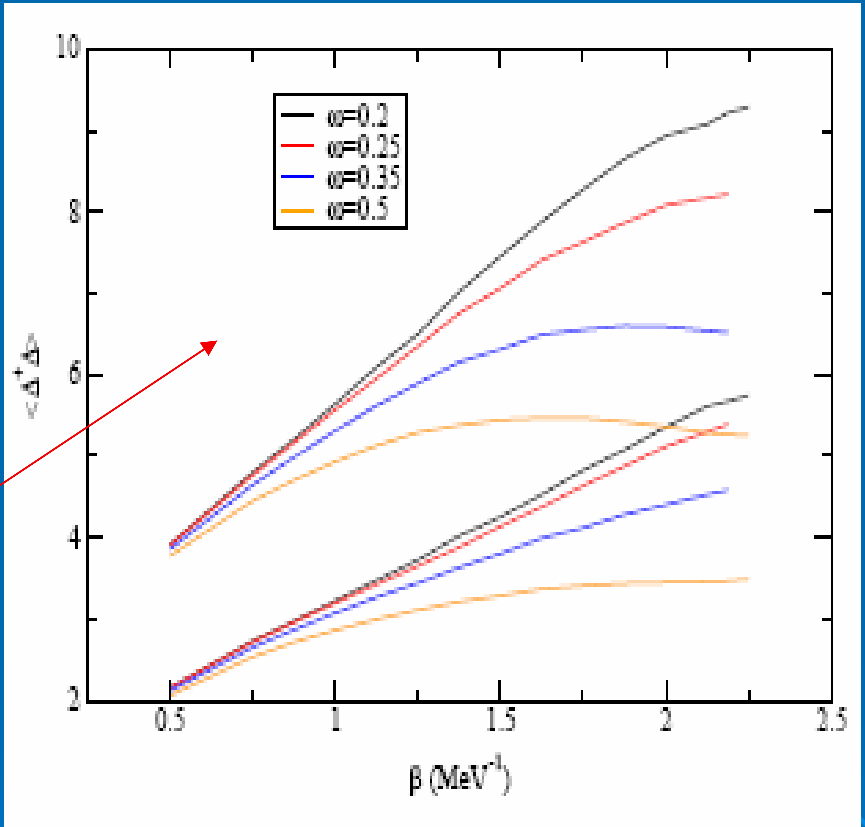
$$I_2 = \frac{d\langle J_z\rangle}{d\omega} = \beta\left(\langle J_z^2\rangle - \langle J_z\rangle^2\right)$$

Occupations

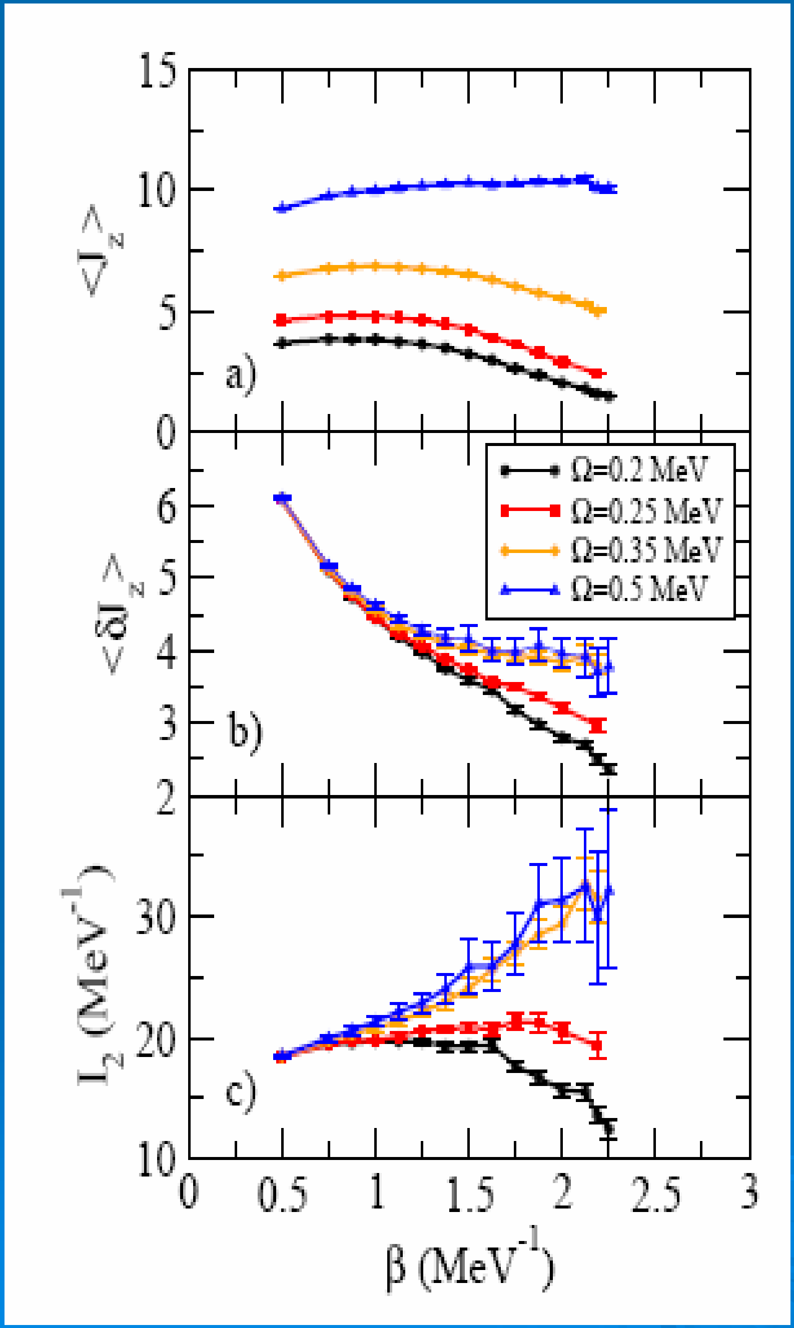


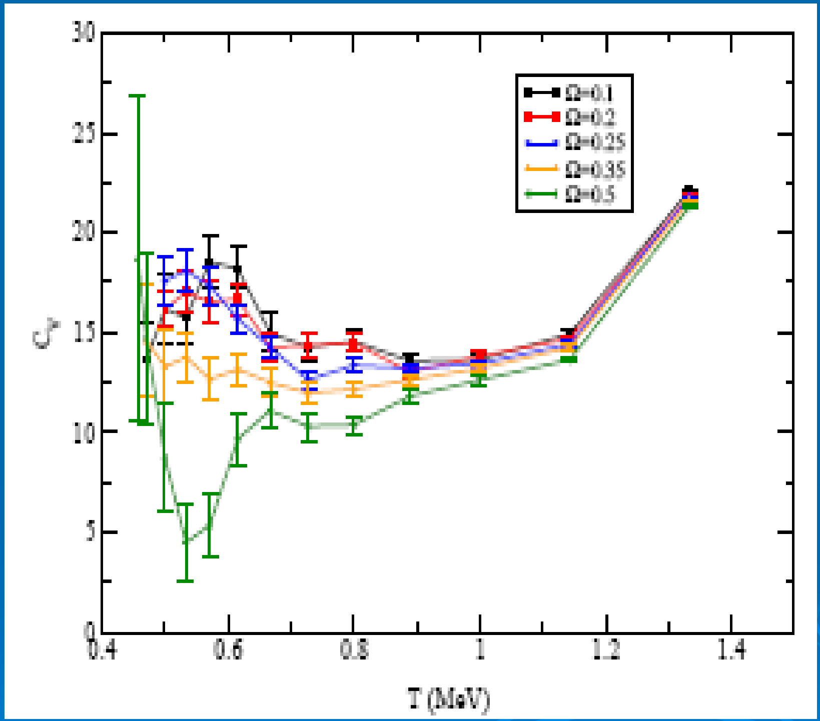
Pairing decreases with increasing frequency





Rotation and temperature in 76-Ge





Conclusions on this section

- Pairing transition tends to occur around T=0.7 MeV with some width due to the finite size of the system.

- Shape transition is more gradual. No peak in the specific heat seen.

- Competition between pairing and shape:
  - Super-fluid systems (Ni-68, static pairing) show a pronounced peak in the specific heat.

  - Strongly deformed nuclei (Zr-80) show a more gradual change the specific heat.

- Major computational effort: each data point is 1 Tf-hour.
- Near term: complete cranking calculations and analysis.

The end….with some quotes:

It is better to know some of the questions than all of the answers.
-- James Thurber

Computers are useless. They can only give you answers.
-- Pablo Picasso

In all things of nature, there is something of the marvelous.
-- Aristotle

Science is facts; just as houses are made of stones, so is science made of facts; but a pile of stones is not a house and a collection of facts is not necessarily science.
-- Henri Poincare

Nothing shocks me. I'm a scientist.
-- Harrison Ford (as Indiana Jones)