# Simplicity and complexity in thestudy of nuclei

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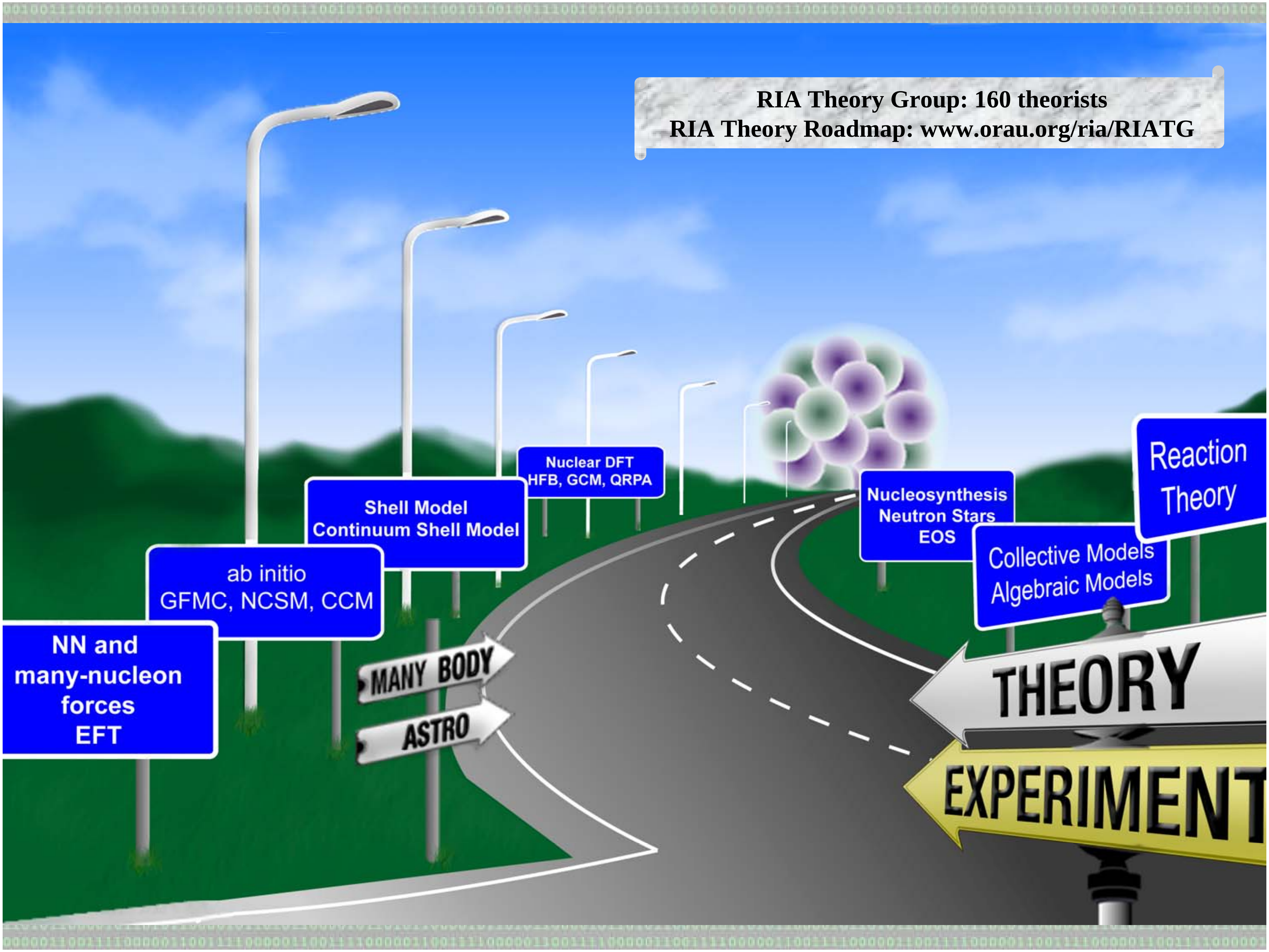
I. The big question:
"Given a lump of nuclear material, what are its properties, where did it come from, and how does it react?"

How are we going to describe nuclei that we cannot measure?
We need robust and predictive nuclear theory.
We need nuclear data to constrain that theory.
Goal: build a unified theory of nuclei

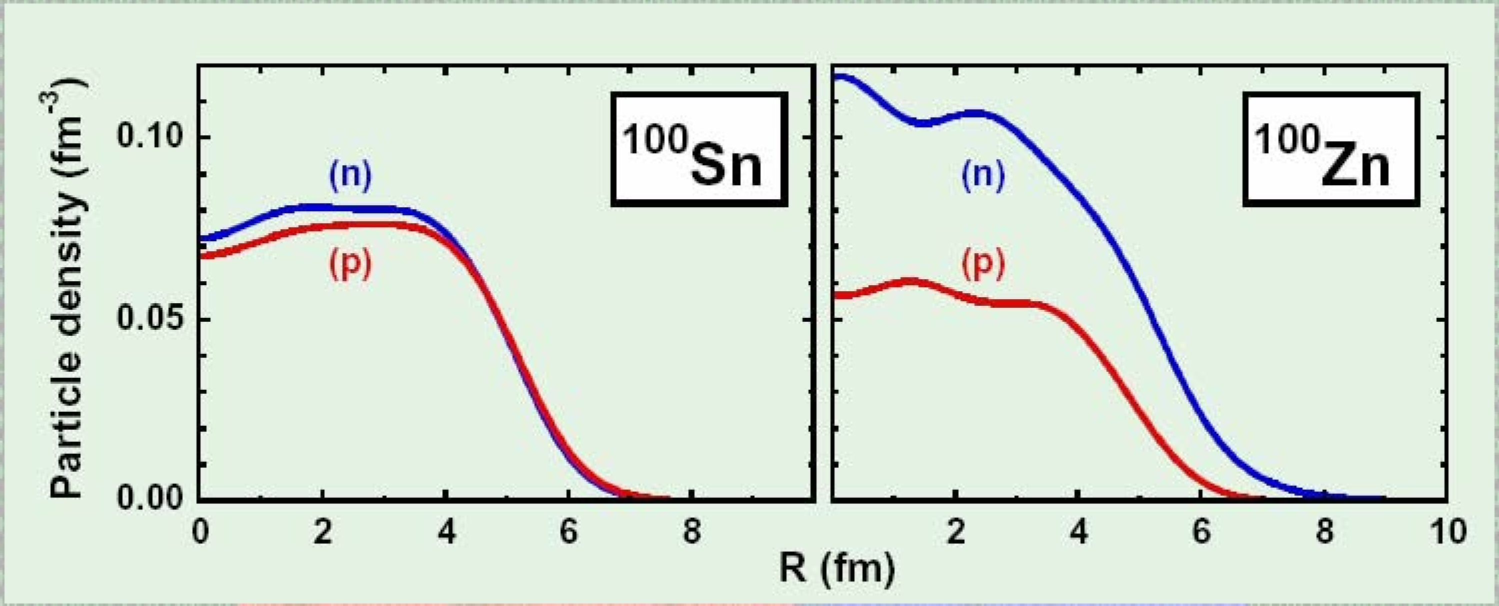
II. Ab initio treatments of nuclei
(building a nucleus from the ground up)

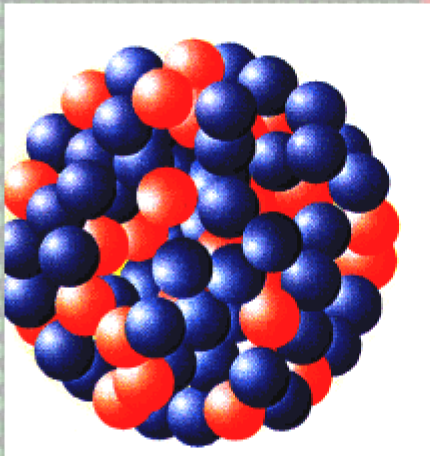
III. Emergent nuclear phenomena
(deformation, pairing, 'magic' numbers…)

IV. Whither RIA? How does physics of exotic nuclei fit into the global U.S. science strategy??


RIA Theory Group: 160 theorists
RIA Theory Roadmap: www.orau.org/ria/RIATG
NN and
many-nucleon
forces
EFT
ab initio
GFMC, NCSM, CCM
Shell Model
Continuum Shell Model
Nuclear DFT
HFB, GCM, QRPA
MANY BODY
ASTRO
Nucleosynthesis
Neutron Stars
EOS
Collective Models
Algebraic Models
Reaction
Theory
THEORY
EXPERIMENT

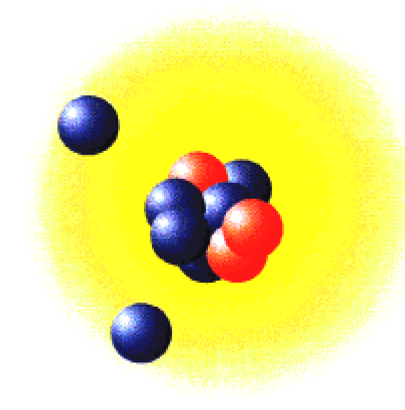
# The challenge of neutron rich nuclei



$^{208}$Pb: Well Bound Heavy Nucleus

| | 'normal' | 'rare' |
|---|---|---|
| Half-life | Long/stable | Short |
| Size | Compact | Halos |
| Continuum | Unimportant | Important |
| Shell closures | Normal magic numbers | New magic numbers |
| Scattering Cross section | 'Normal' | Enhanced |



$^{11}$Li: Borromean Halo Nucleus

# Chiral Perturbation theory

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

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

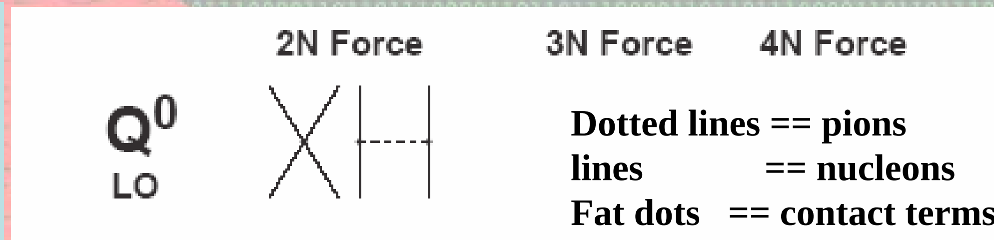
Lagrangian
→ infinite sum of Fe

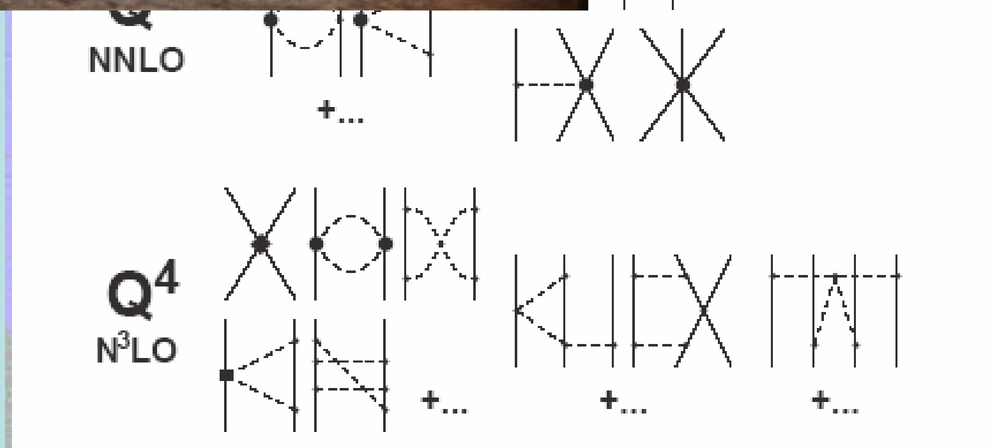
Expand in $O(Q/\Lambda_{QCD})$

Weinberg, Ordonez, Ray, van Kolck

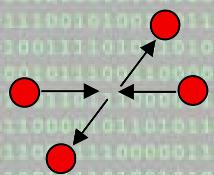
NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

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



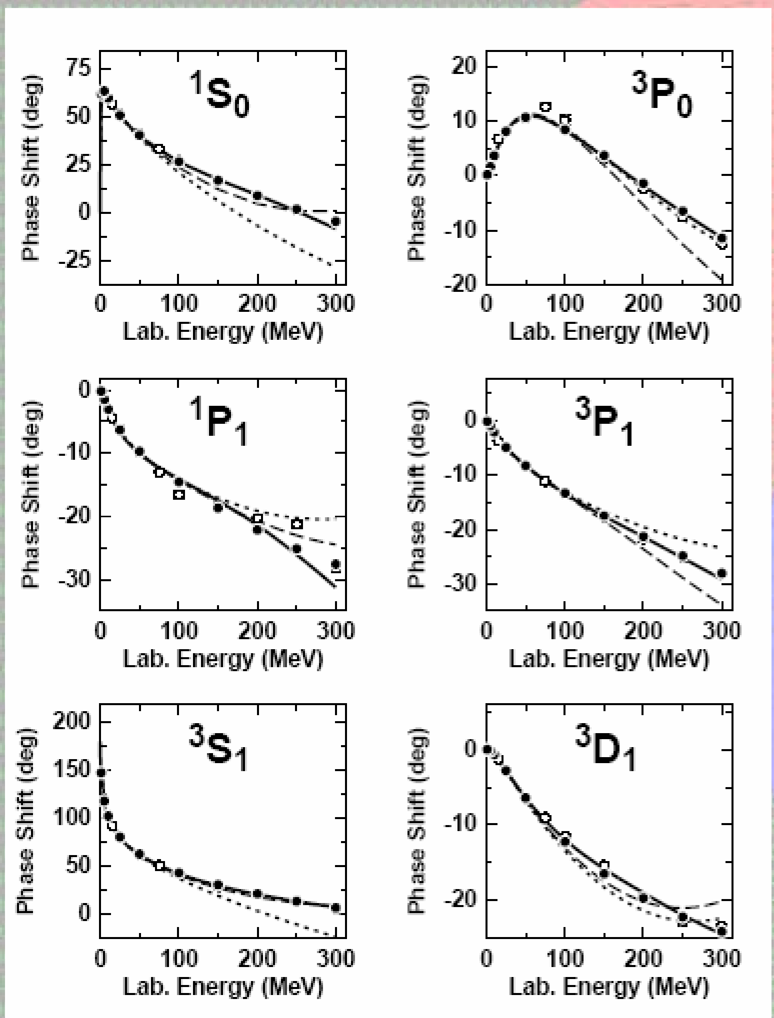

# Nuclear interactions: Cornerstone of the entire theoretical edifice

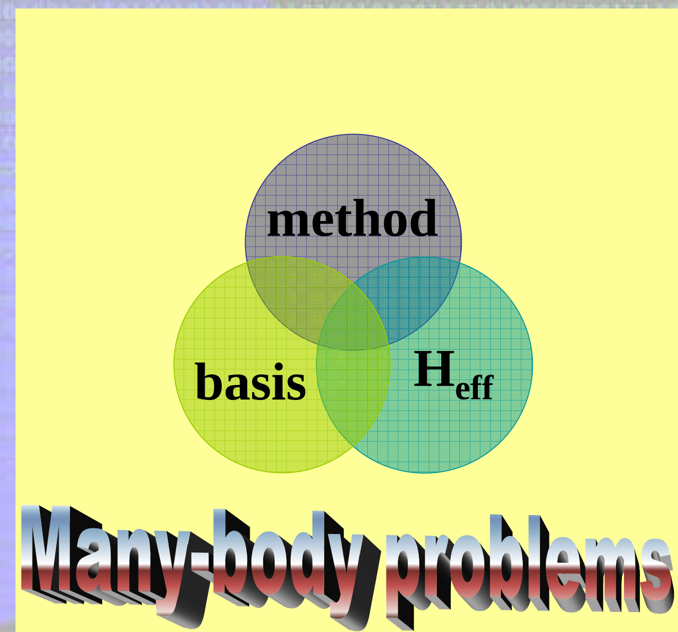


$$H = \sum_{i=1,A} \frac{-\hbar^2}{2M_i} \nabla_i^2 + \sum_{i<j} V(r_i, r_j) + V_{NNN}$$

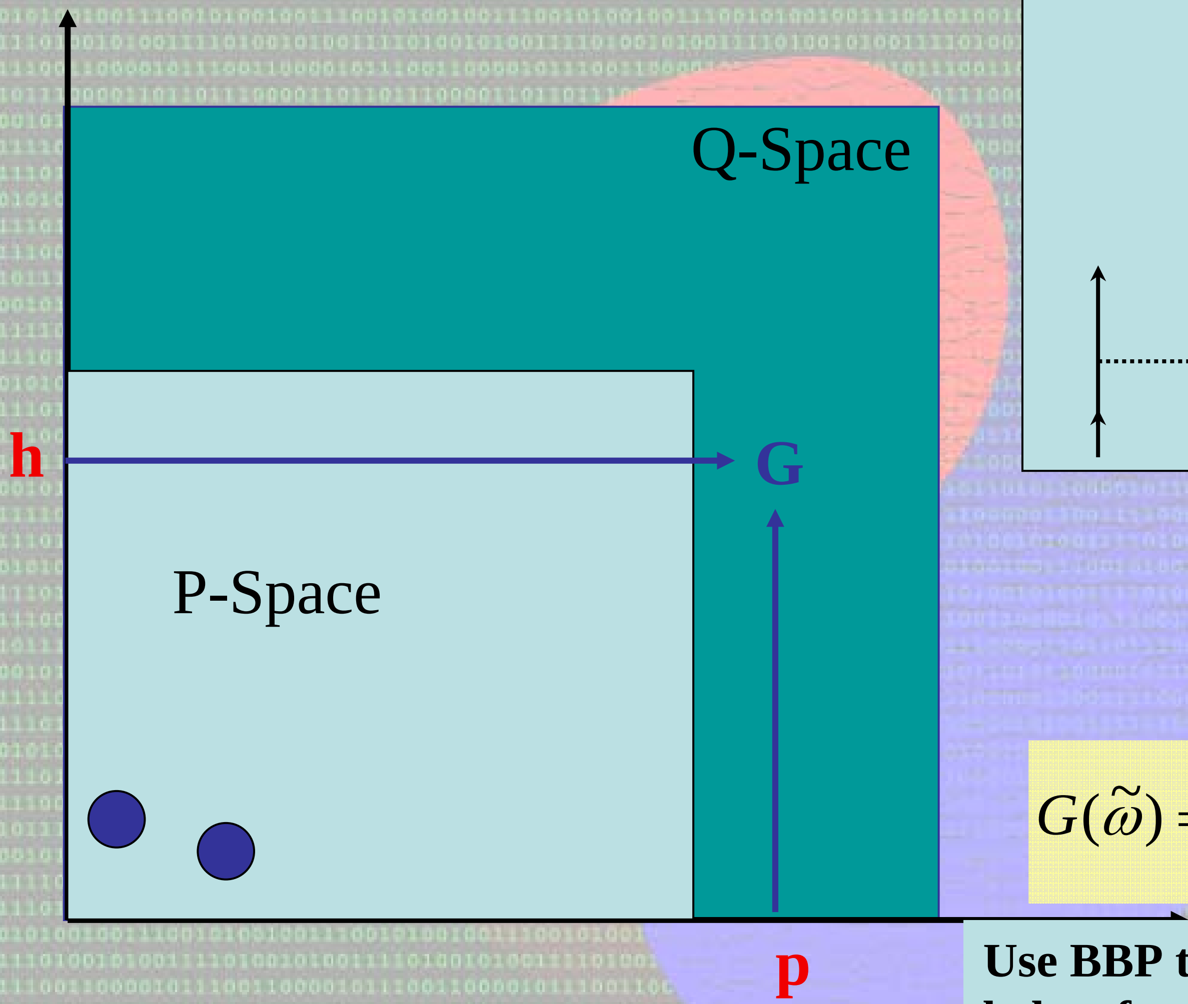
→ **Bare (GFMC)**

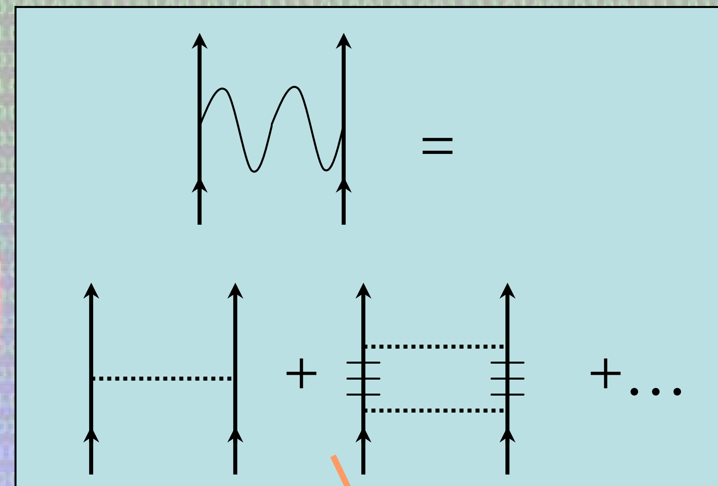
→ **Basis expansion**



# 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.**

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

## 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**

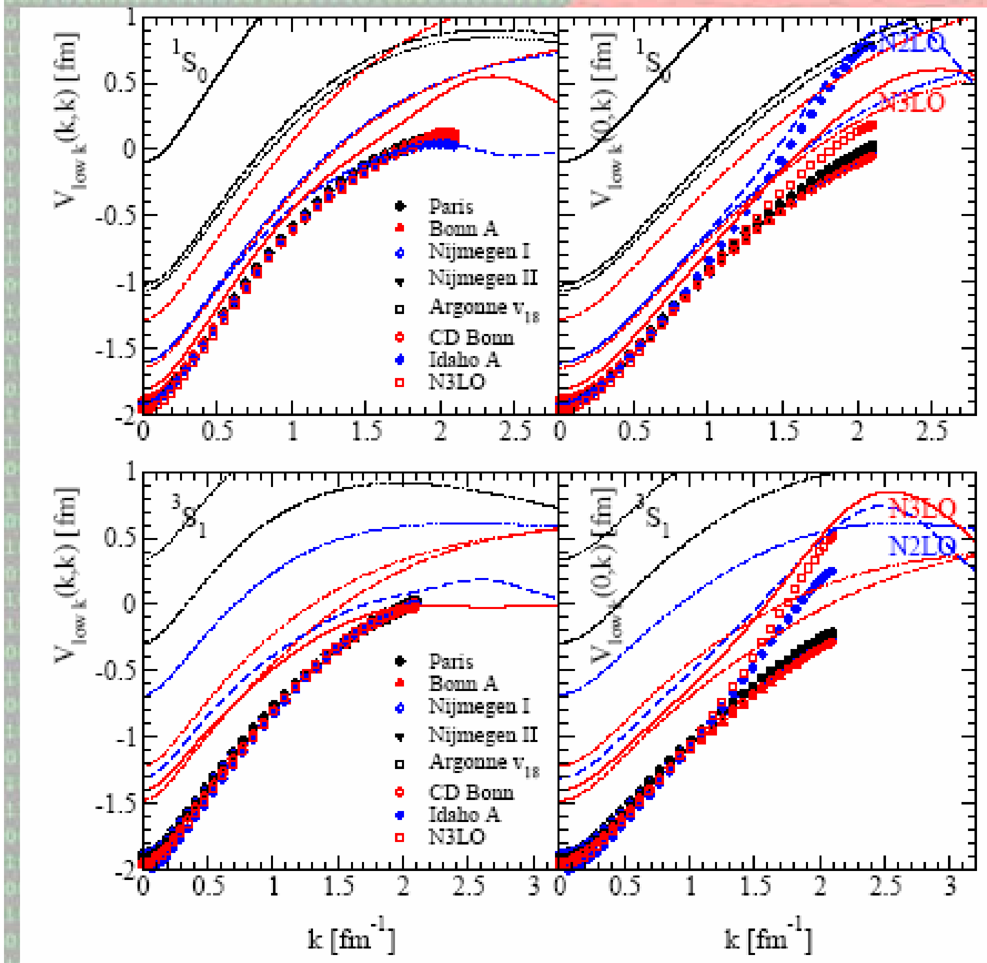
**Current status**

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

# Another approach: $V_{lowk}$

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

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




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

**Method due to Schwenk, Bogner, Brown, Kuo**

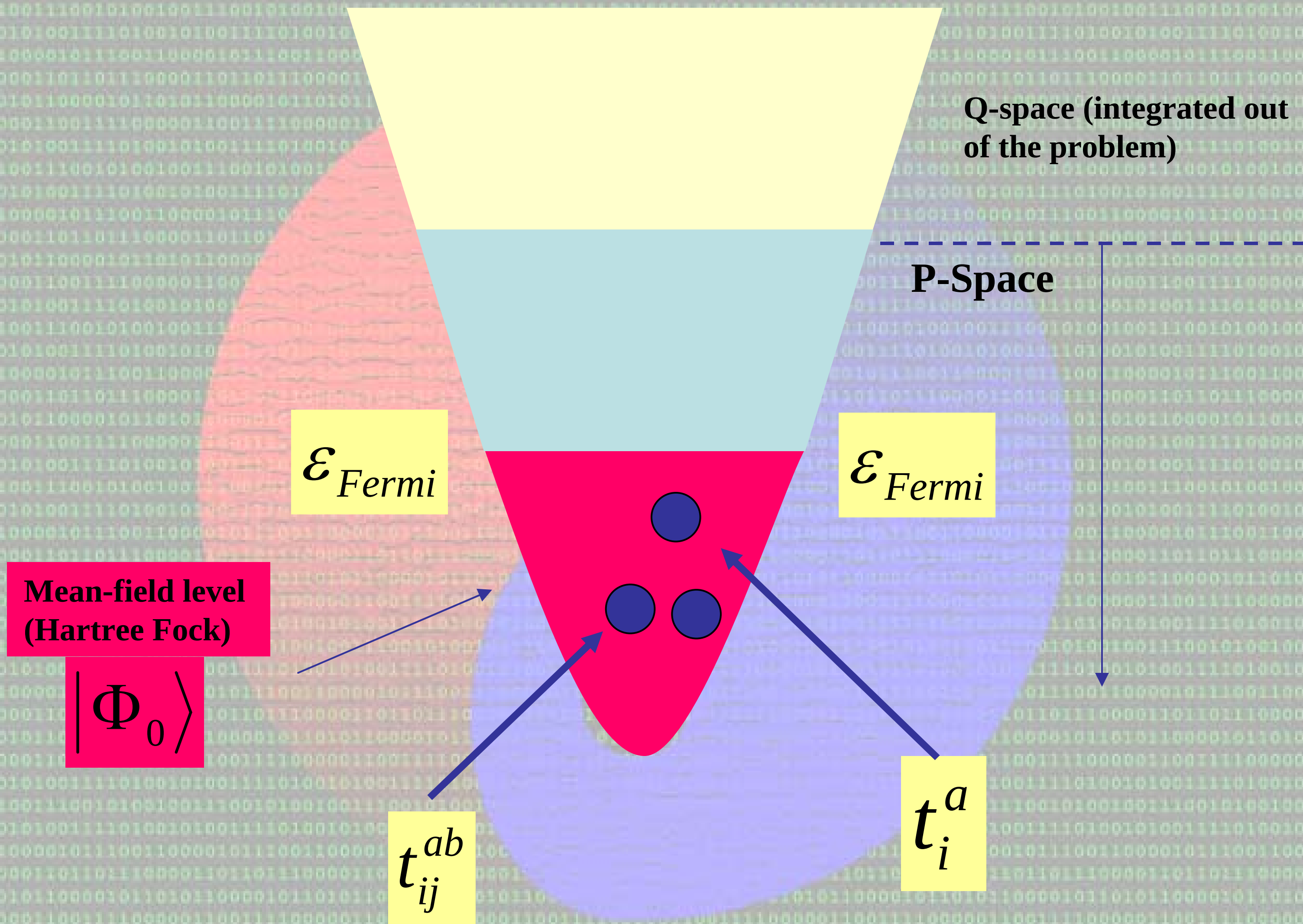
**Produces a phase-equivalent potential that may then be used in many-body calculations.**

**The potential over binds.**

**Must be augmented by a 3-body force.**

**This approach does engender controversy, but it is an interesting one to investigate.**

# Interactions within the P-space




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

# 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

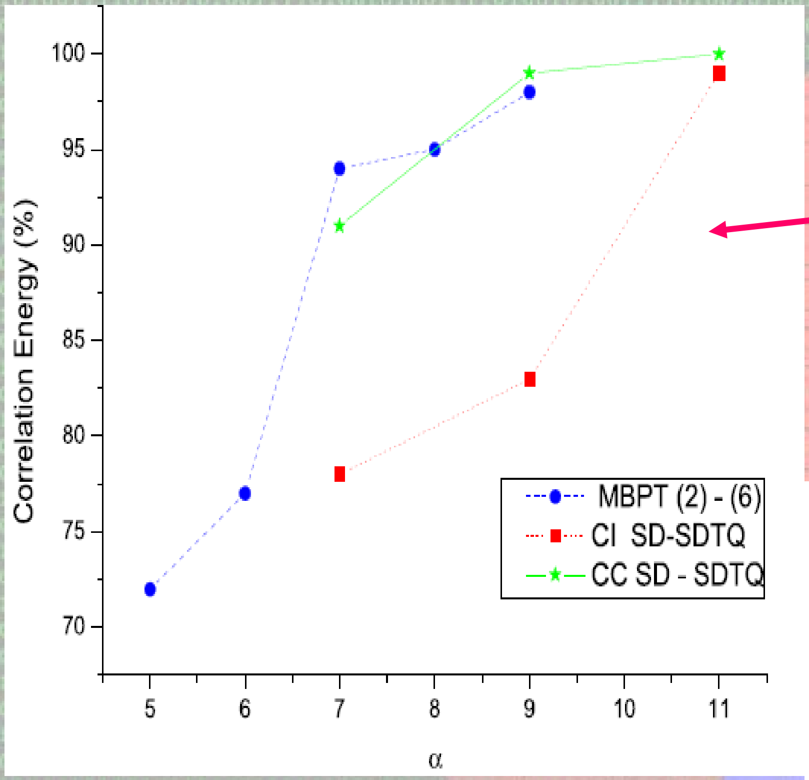
$$E = \left\langle\Phi\right|\exp(-T)H\exp\left(T\right)\left|\Phi\right\rangle$$

## Amplitude equations

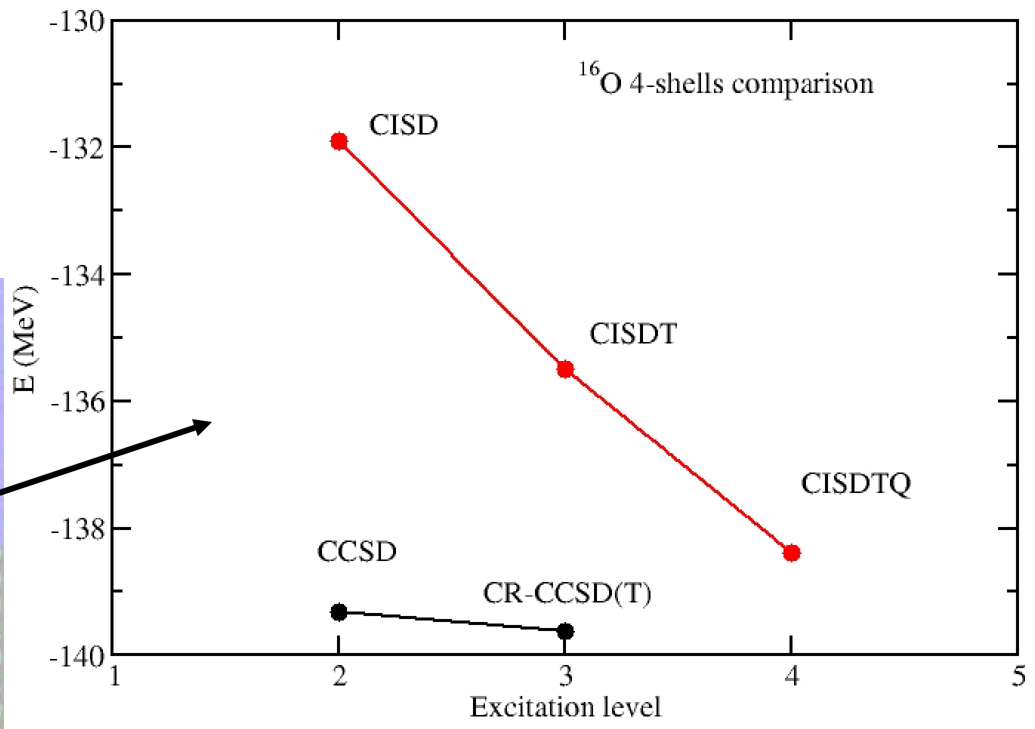
$$\left\langle\Phi_{ij\cdots}^{ab\cdots}\right|\exp(-T)H\exp\left(T\right)\left|\Phi\right\rangle = \left\langle\Phi_{ij\cdots}^{ab\cdots}\right|\overline{H}\left|\Phi\right\rangle = 0$$

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

# Comparisons with other many-body techniques

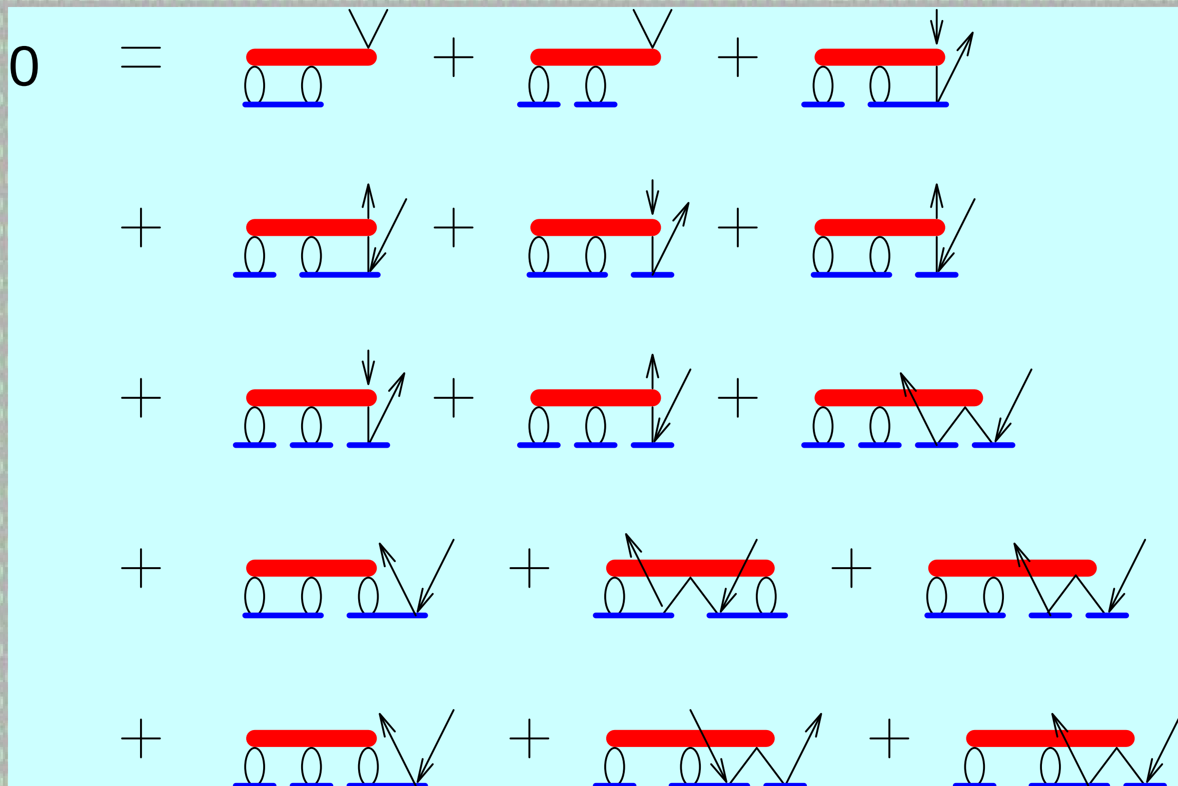



Quantum chemistry example (Bartlett et al)



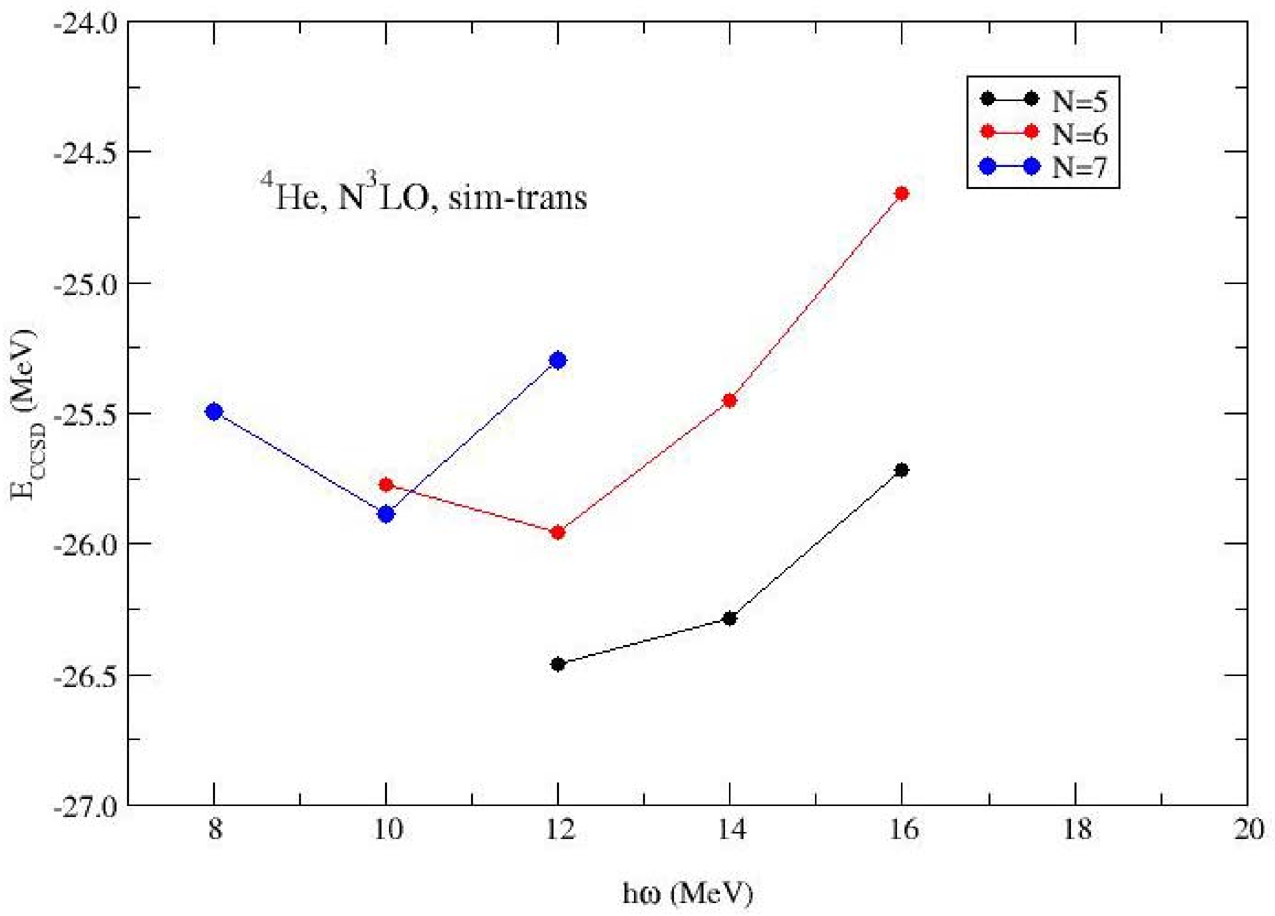

Nuclear Example (Kowalski et al PRL 2004).

# Inclusion of three-body forces:




**Results with three-body forces included coming soon…..**

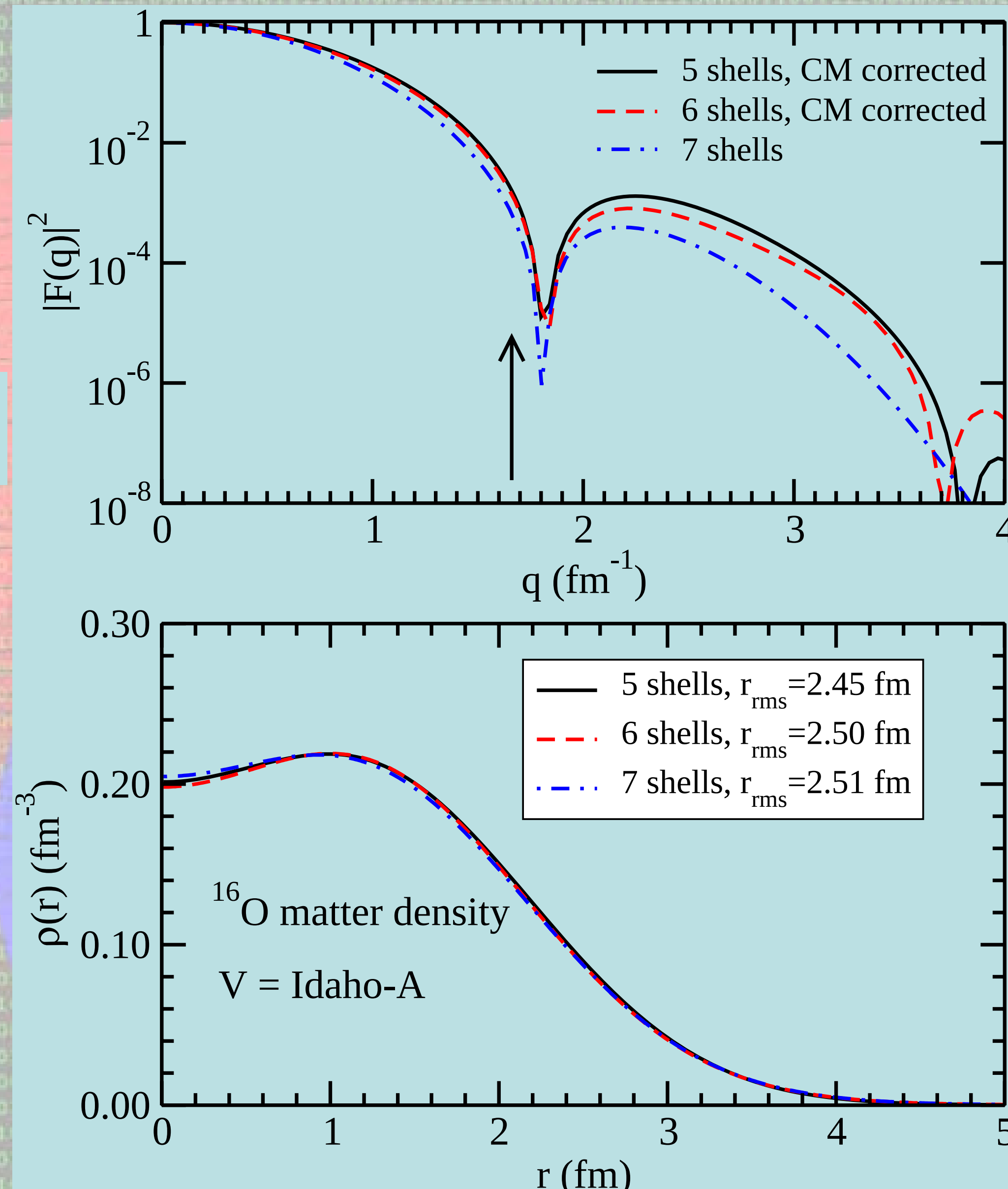
# Using the similarity tranform: $H=T-T_{cm}+V$



# Nuclear Properties

$$\rho_{\alpha\beta} = \left\langle \Phi \middle| L^{(\mu)} \left[ e^{-T} a_\alpha^+ a_\beta e^T \right] R^{(\mu)} \middle| \Phi \right\rangle$$

**Also includes second-order corrections from the two-body density.**



# 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. $H \leftarrow T + V - \langle T_{cm} \rangle$

| $J^\pi$ | Expt. | $N^3LO$ | 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 |

**BE/A**

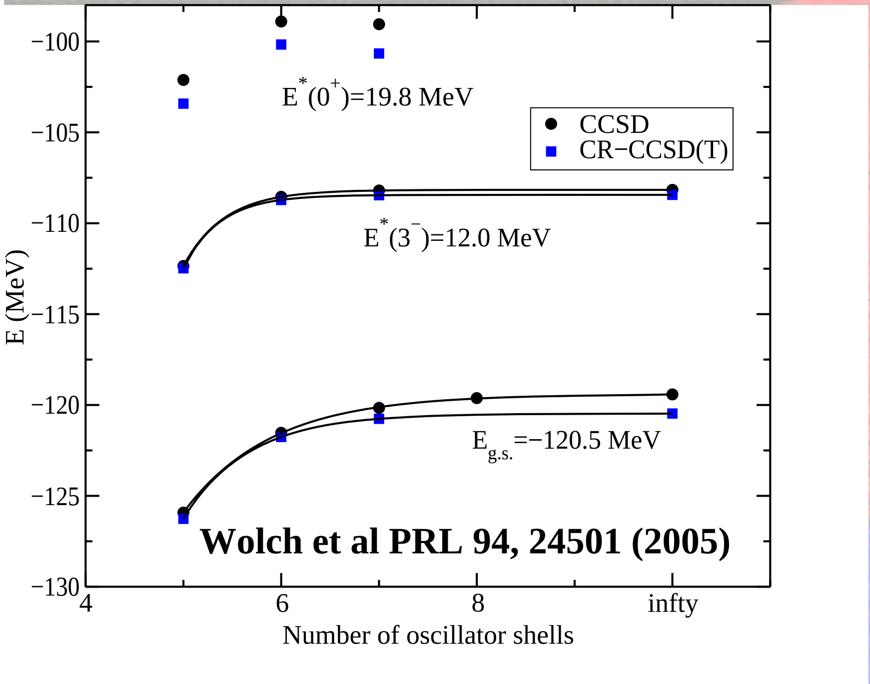
| $J^\pi$ | Expt. | $N^3LO$ | CD-Bonn | AV18 |
|---|---|---|---|---|
| $3/2^+$ | 5.085 | 5.68 | 6.41 | 3.946 |
| $1/2^+$ | 0.870 | -0.088 | 0.31 | -0.390 |
| $5/2^+$ | 0.0 | 0.0 | 0.0 | 0.0 |

**$^{17}O$, all MeV**

| $J^\pi$ | Expt. | $N^3LO$ | CD-Bonn | AV18 |
|---|---|---|---|---|
| $3/2^-$ | 6.176 | 6.26 | 7.35 | 4.452 |
| $1/2^-$ | 0.0 | 0.0 | 0.0 | 0.0 |

**$^{15}O$, all MeV**

# 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**

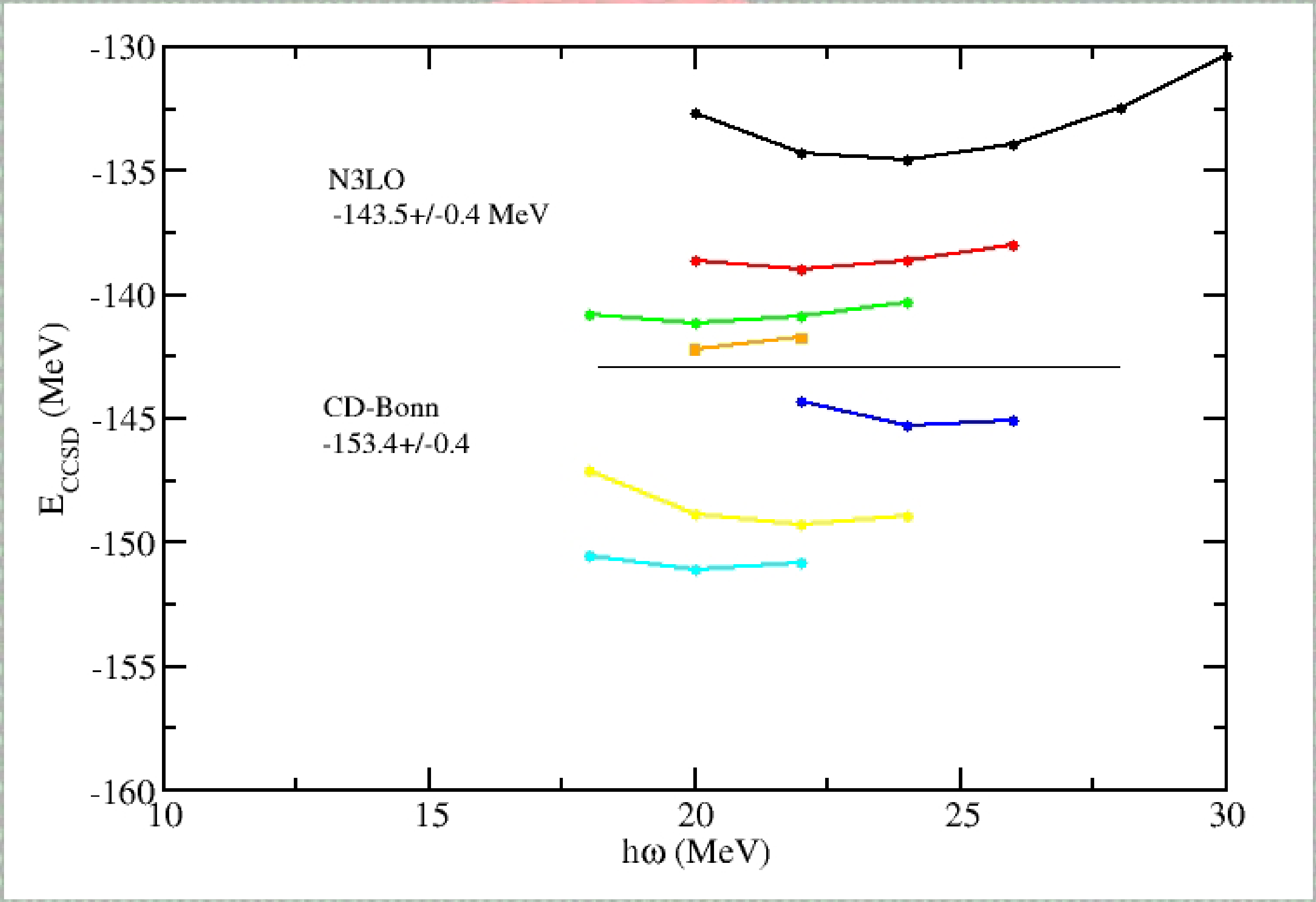
**From CCSD**

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

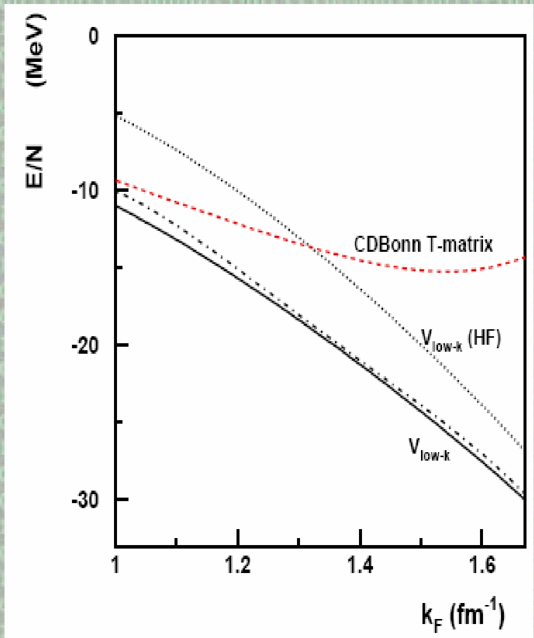
**Interactions among nucleons lowers by about 15.8-11.5=4.3 MeV**

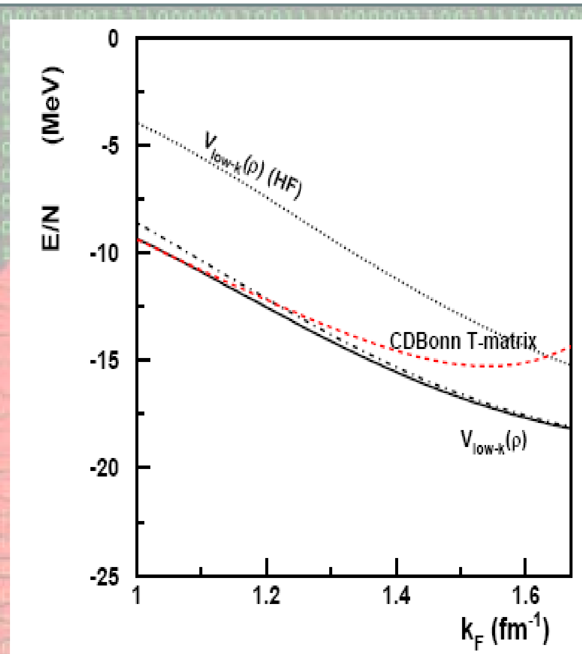
**Much of the discrepancy comes from where the interaction places the 0p shell relative to the 0d1s shell.**

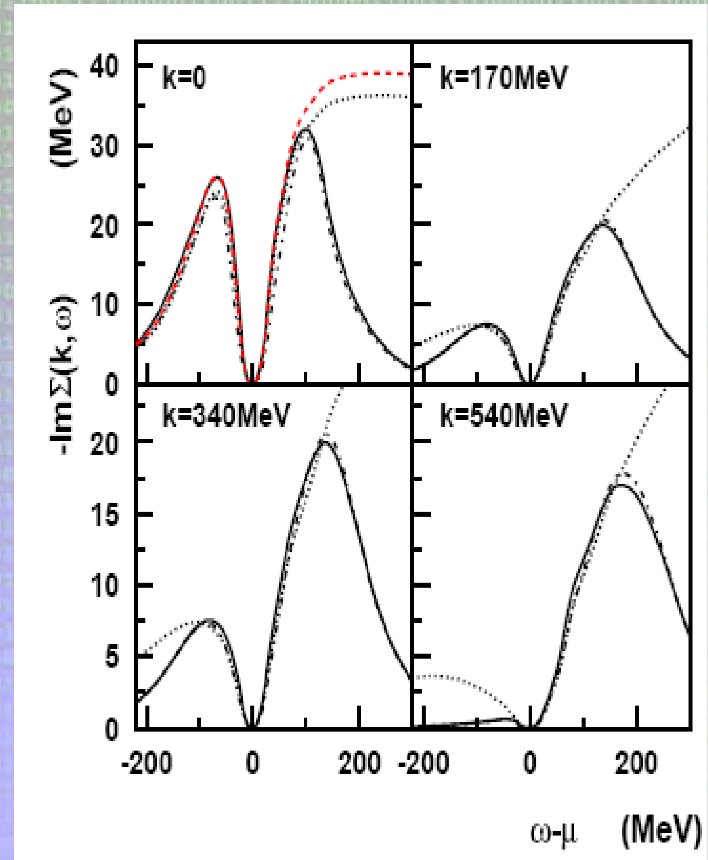
# $V_{lowk}$ $^{16}O$ results using N3LO and CD-Bonn

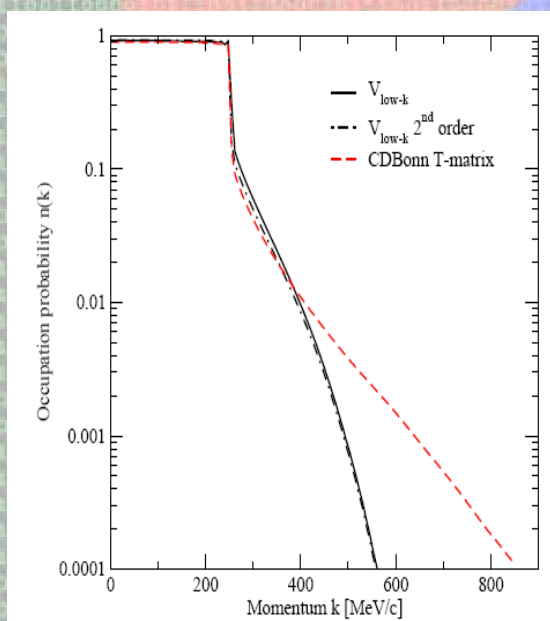


# Some studies of $V_{lowk}$ in nuclear matter



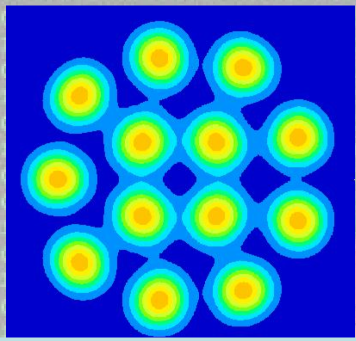




**Bozek, Dean, Muether, PRC submitted**

# Emergent phenomena

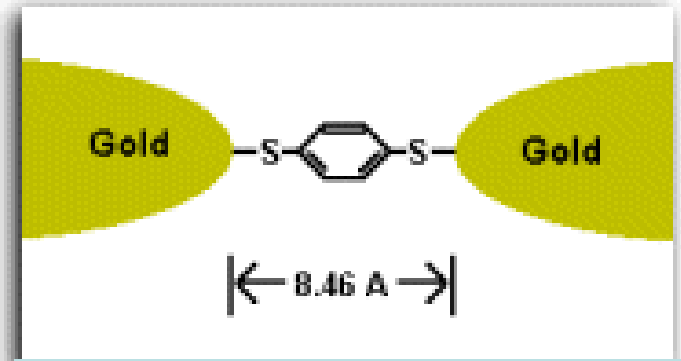
**Nanoscale**

~10 nm



2-d quantum dot
in strong magnetic field.
The field drives localization.

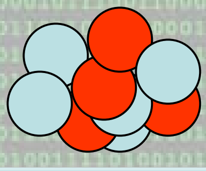
**Molecules**




Molecular scale: conductance
through molecules.
Delocalized conduction orbitals

**Nuclei**

~7 fm



- Studies of the interaction
- Degrees of freedom
- Astrophysical implications

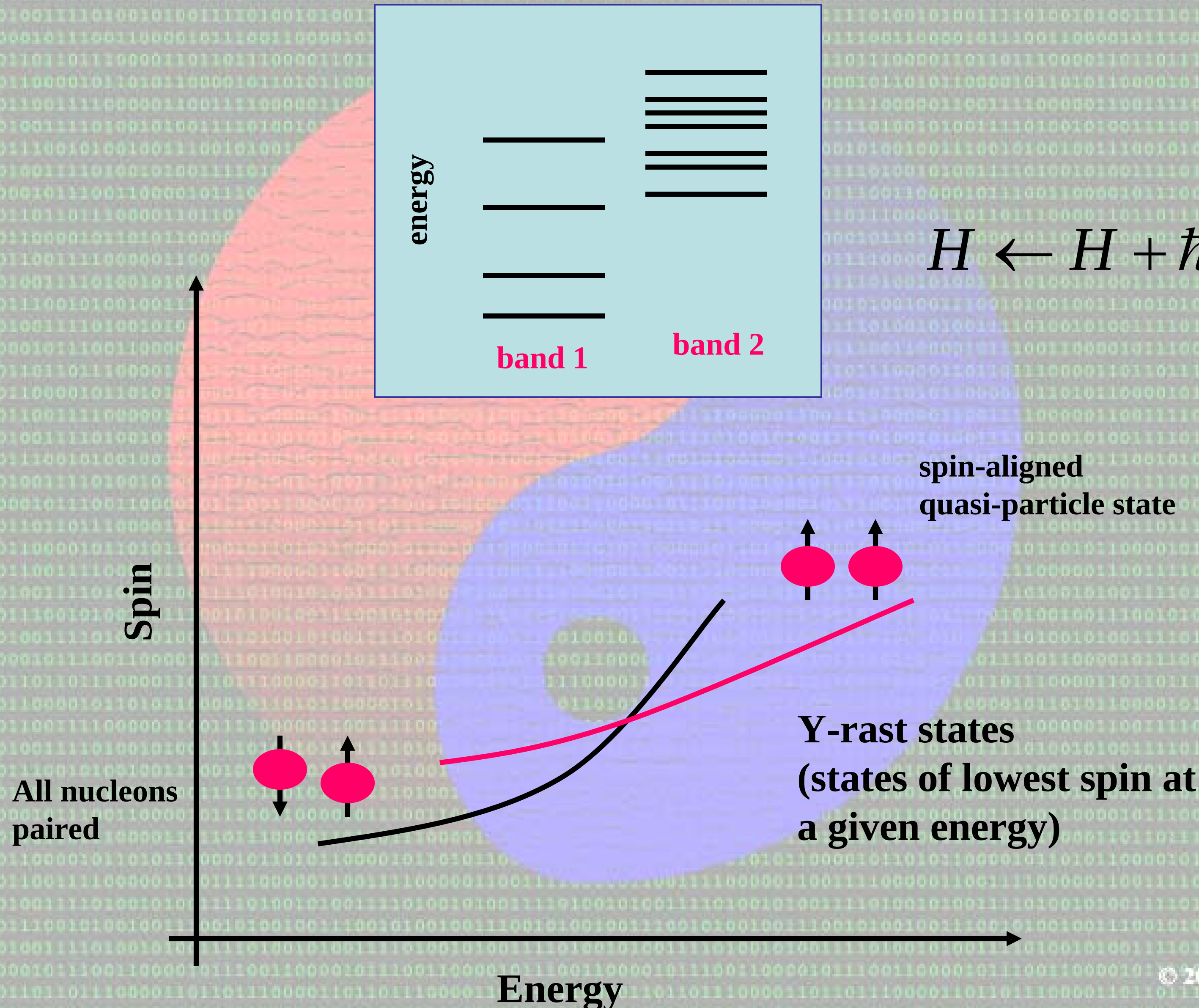
Quantum mechanics plays a role when the size of the object is of the same order as the interaction length.

**Common properties**

- Shell structure
- Excitation modes
- Correlations (superfluidity)
- Phase transitions
- Interactions with external probes

# What happens to pairing in a (hot) rotating nucleus?

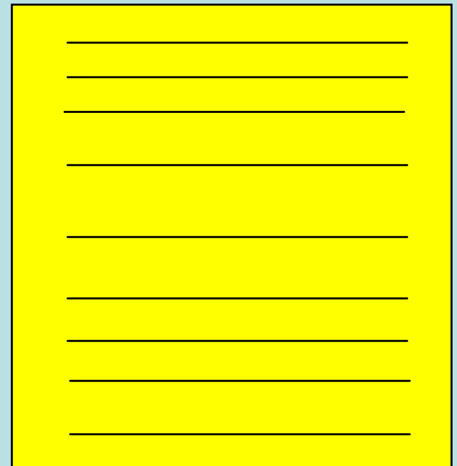
$$H \leftarrow H + \hbar\omega J_z$$



# 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**

# 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**

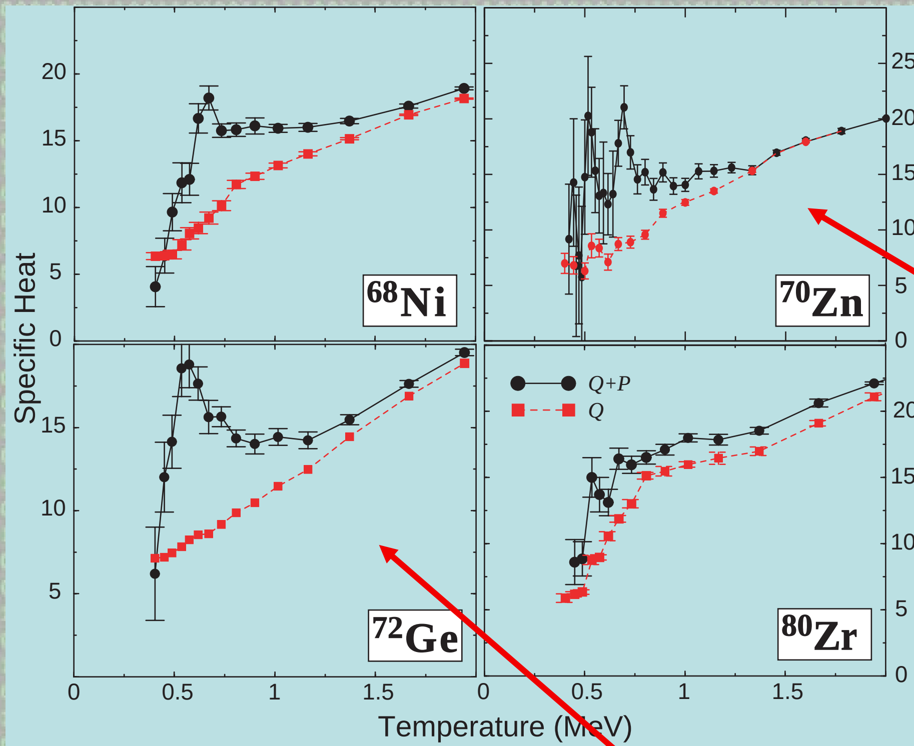
$$\exp\left(-\beta\hat{H}\right) = \sqrt{\frac{\beta|V|}{2\pi}}\int_{-\infty}^{\infty} d\sigma \exp\left(-\beta|V|\sigma^2/2\right)\exp\left(-\beta\hat{h}\right)$$

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

$s = 1 \quad \mathit{for} \quad V < 0$

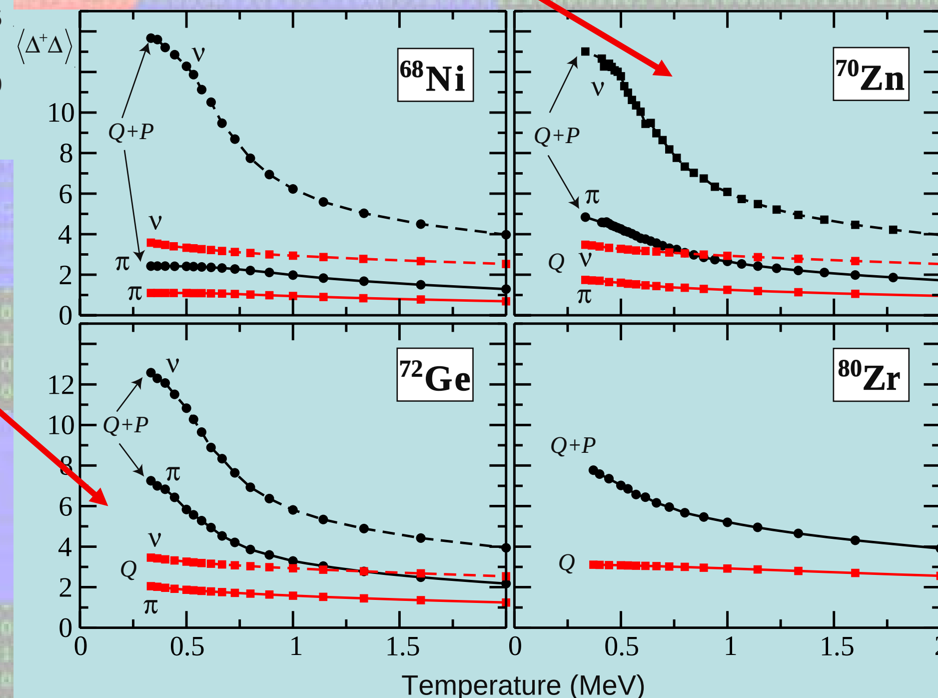
$s = i \quad \mathit{for} \quad V > 0$

# Pairing, deformation, and the specific heat



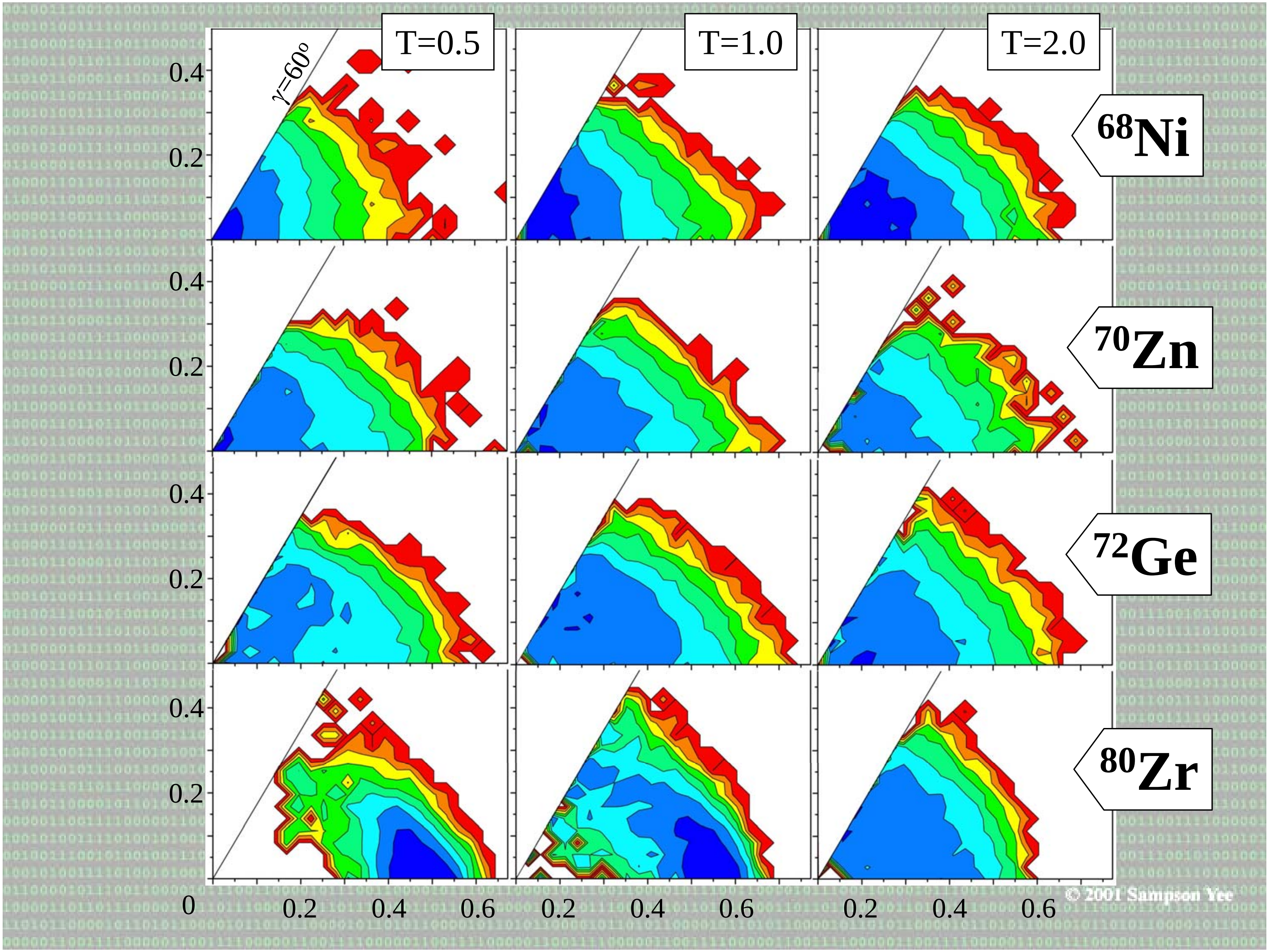

$$E(\beta) = \frac{Tr\left[\exp(-\beta H)H\right]}{Tr\left[\exp(-\beta H)\right]}$$

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

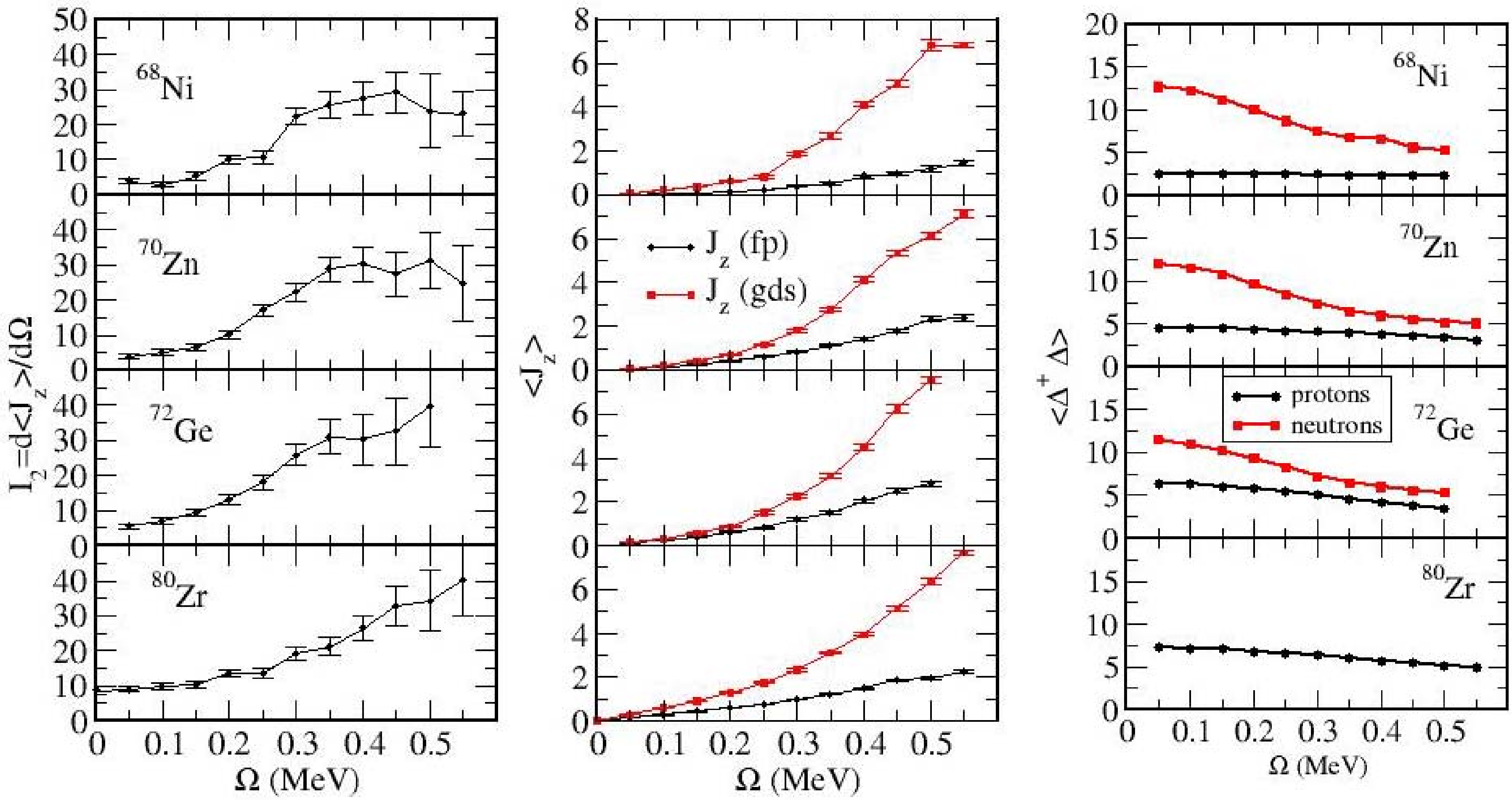





Langanke, Dean, Nazarewicz (NPA, 2005)

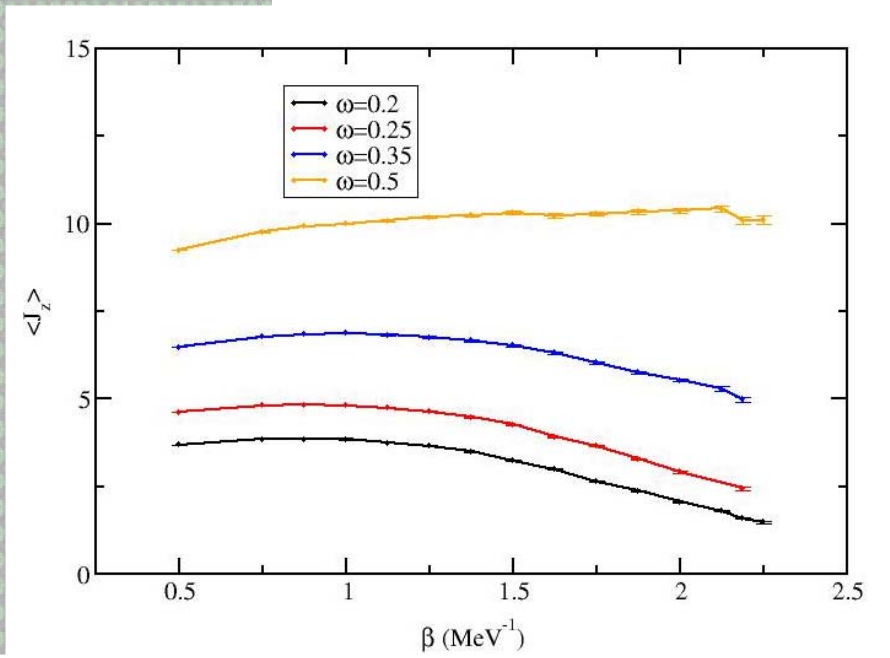

T=0.5
T=1.0
T=2.0
γ=60°
$^{68}$Ni
$^{70}$Zn
$^{72}$Ge
$^{80}$Zr
0.4
0.2
0
0.2
0.4
0.6
© 2001 Sampson Yee

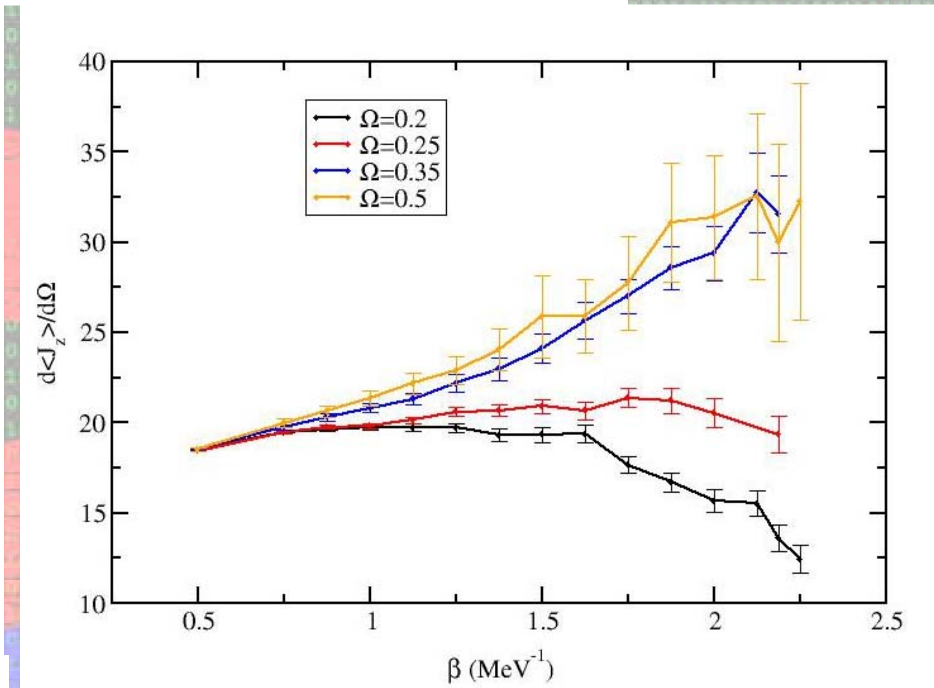
# Low temperature and rotation

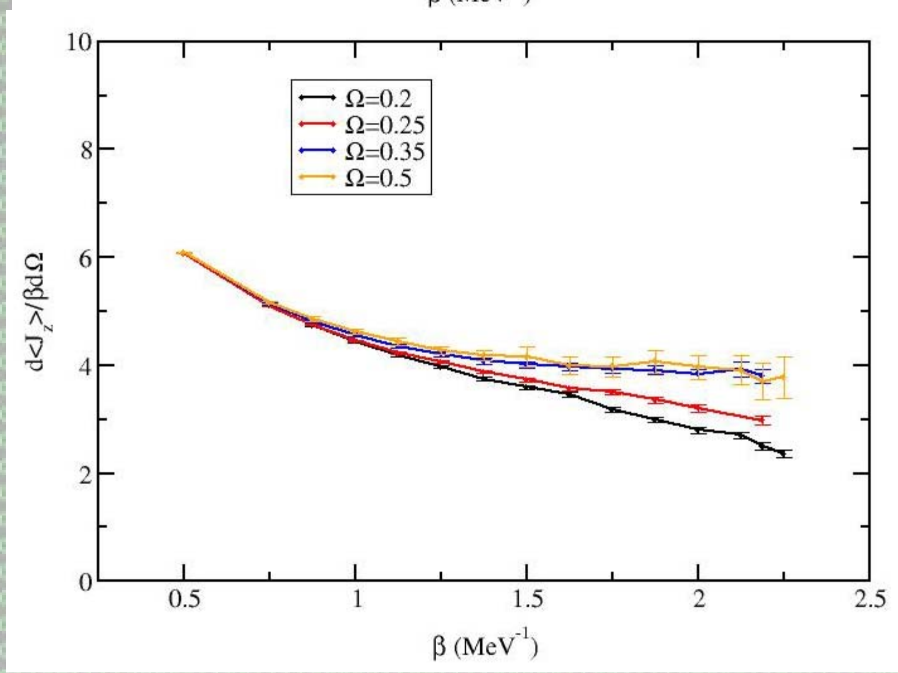


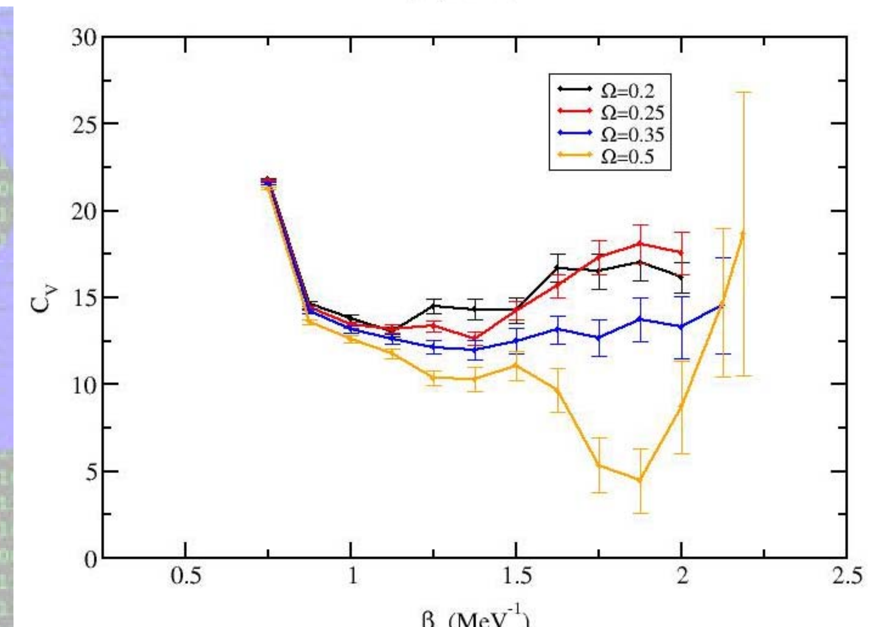

Dean, Nazarewicz, Langanke (in prep)

# Interplay between rotation and temperature



## What questions does your research pose that only "RIA" can answer?

**I prefer to take the long view on this question…..**

# President's Council of Advisors on Science and Technology (PCAST): 28 March 2006

**Marburger …the American Competitive Initiative is keyed to research that will promote competitiveness…. Concerning DOE Office of Science programs, he commented that high energy physics and nuclear physics research are important and cited societal contributions they have made.…But DOE's Basic Energy Sciences program is key, Marburger said, as its research is closely aligned with competitiveness.**

**Bodman's remarks reinforced these comments…"The ACI is the significant investment needed to produce transformational technologies to help us achieve the President's goals."**

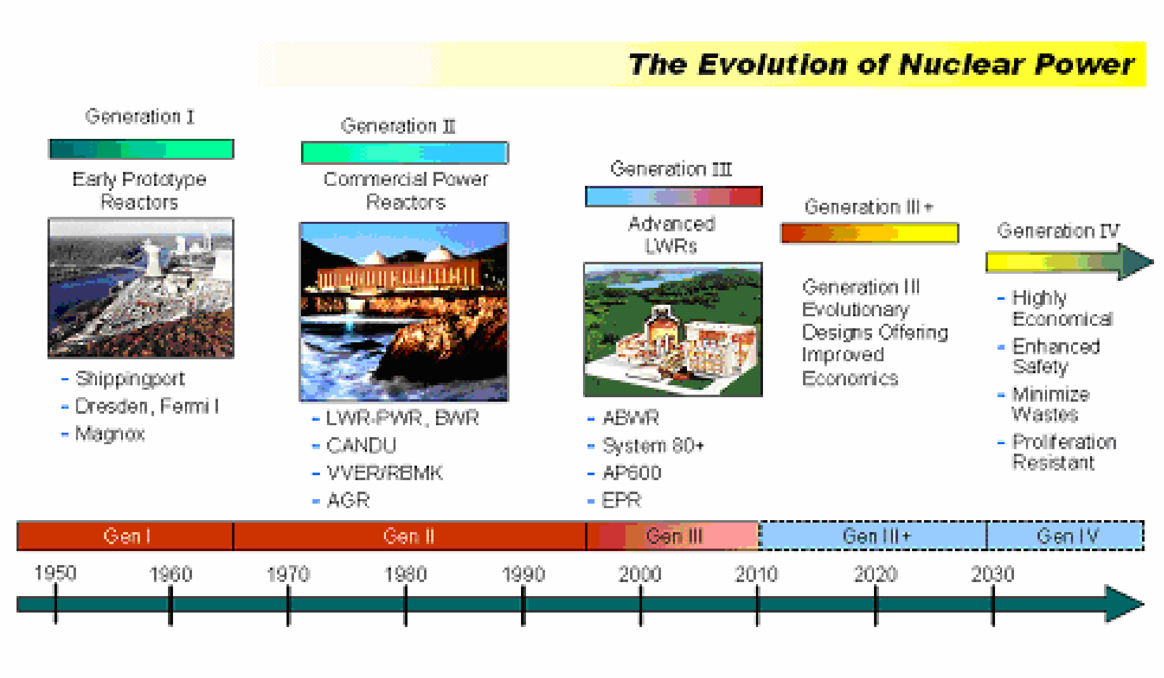
**After discussing DOE's proposed work in ethanol production and the Global Nuclear Energy Partnership, Bodman reiterated…: "The American people, the taxpayers, expect more from basic science research than new knowledge alone. We expect and I believe that the investments being made today will one day result in countless additional benefits -- benefits to our health, our national defense, our productivity and economic expansion, and our energy security."**

# Global Nuclear Energy Partnerships

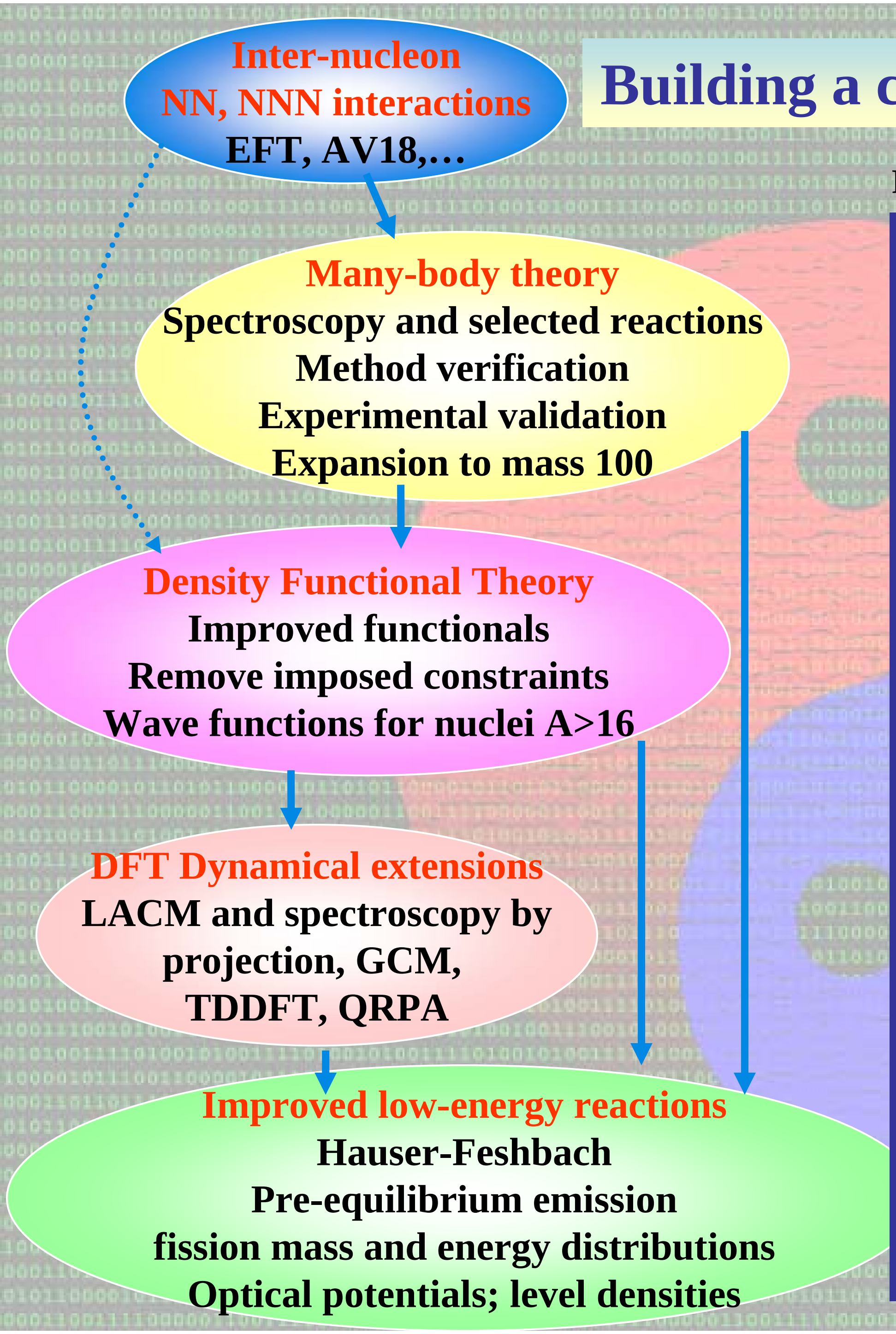
**The Advanced Burn Reactor recycles used nuclear fuel**

**The ABR would destroy transuranics in used fuel from nuclear power plants, avoiding the need to accommodate this radioactive, radiotoxic, and heat-producing material in a geological repository for hundreds of thousands of years while it decays.**

**To "burn" this material, an ABR takes advantage of high-energy or fast neutrons to fission … transuranics. Here, "burn" means to transmute or convert transuranics into shorter-lived isotopes. As transuranics are consumed, significant energy is released and converted into electricity, hereby producing useful energy from material that would otherwise be waste.**



# 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**

# Kovar presentation, NSAC March, 2006

U.S. Department of Energy
Office of Science

## FY 2007-2011 Nuclear Physics Program
## Impacts / Implications

*Facility Operations*

- Operate and implement the capabilities of the user facilities (RHIC, CEBAF, HRIBF and ALTAS) to achieve their scientific goals.
  - Proceed with the 12 GeV CEBAF Upgrade project.
  - RHIC accelerator/detector upgrades implemented and RHIC II construction starts midway in period
  - ATLAS and HRIBF research capabilities are developed to mount forefront programs.
  - R&D is supported to provide the basis for a decision to initiate preliminary engineering design at the end of this planning period for construction of a U.S. world-class exotic beam facility.

*Research*

- Research efforts and investments are supported to achieve the scientific goals and address highest priority new scientific opportunities
  - CEBAF 6-GeV program will be completed with several key experiments
  - RHIC program will characterize the newly discovered new states of matter with heavy ion beams and establish the contributions of gluons to the spin of the proton using a polarized beams
  - U.S. researchers at LHC will search for new states of matter at conditions different than RHIC
  - Studies of new nuclear structures and nuclear behaviors start with GRETINA
  - Measurements of fundamental neutron properties will begin at the FNPB at SNS
  - A neutrinoless Double Beta Decay experiment is fabricated
  - Investments in LQCD (with HEP) will provide the opportunity for unprecedented advances.
  - Accelerator R&D for next-generation nuclear physics research capabilities are supported.
  - Nuclear data measurements and code development will contribute to improved designs of next generation nuclear reactors
  - Support of graduate students will result in over 400 PhD degrees over this period

- **RIA is no longer in the President's budget**
- **Reaccelerated Exotic Beam R&D is in the budget**
- **RISAC (NAS) is evaluating the scientific case for Rare Isotope Physics**
- **That scientific case has been formulated many times. It will need retuning for the future without RIA.**

**Exotic Beam physics remains a key capability of the future DOE scientific portfolio.**