Nuclear Structure II: From the NN Interaction to the Shell Model

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Outline

1. NN
2. GFMC:
   - Green's Function Monte Carlo
3. NCSM:
   - No-Core Shell Model
4. RSM:
   - Regular Shell Model

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The NN Interaction

Let's try to model it as a traditional non-relativistic potential.

Example: Argonne v18

$$v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{R}$$

Electromagnetic term comes from QED. One-pion-exchange part differentiates between neutral and charged pion exchange:

$$v_{ij}^{\pi} = \text{const.} \left[m_0^3 X_{ij}^0 \tau_i^z \tau_j^z + m_{\pm}^3 X_{ij}^{\pm} (\vec{\tau}_i \cdot \vec{\tau}_j - \tau_i^z \tau_j^z) \right] \; ;$$

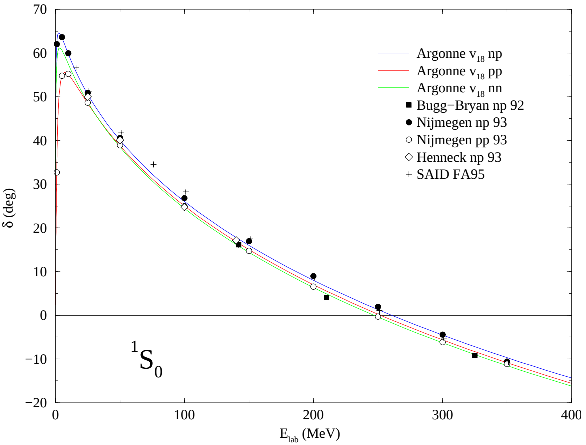
$$X_{ij}^m \approx \frac{e^{-m r_{ij}}}{r_{ij}} \left[\vec{\sigma}_i \cdot \vec{\sigma}_j + \left(\frac{3}{m r_{ij}^2} + \frac{3}{m r_{ij}} + 1 \right) (3(\hat{\mathbf{r}}_{ij} \cdot \sigma_i)(\hat{\mathbf{r}}_{ij} \cdot \sigma_j) - \vec{\sigma}_i \cdot \vec{\sigma}_j) \right]$$

The rest (v_{ij}^R) is two-pion and heavy-meson exchange and contains about 40 adjustable parameters. Depends on orbital angular momentum as well as radial distance, spin and isospin.

Fitting the Parameters

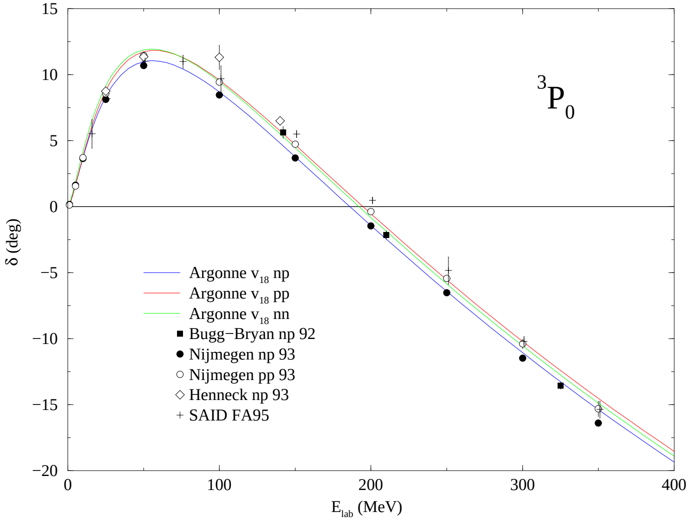
Potential fitted to

- 1787 pp and 2514 np phase shifts for $E = 0 - 350$ MeV
- nn scattering length
- deuteron binding energy



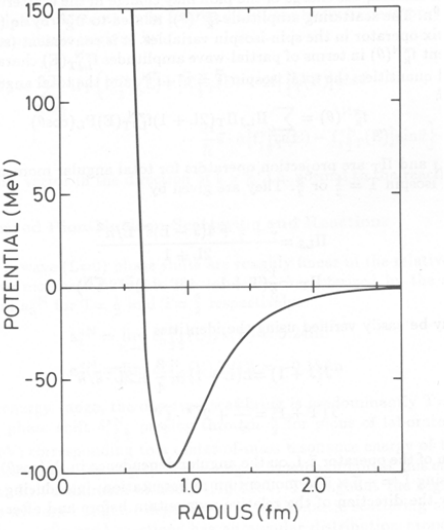
From http://www.phy.anl.gov/theory/research/av18/index.html

Another Partial Wave...



Roughly What It Looks Like:

From E. Ormand, http://www.phy.ornl.gov/npss03/ormand2.ppt



Note "hard core" at $r \lesssim .6$ fm.

Prevents nucleons from getting close. Other equally good model potentials have hard cores that differ significantly from Argonne's because when nucleons get closer they can excite internal degrees of freedom that we don't completely understand. so...

How real is the hard core?

Even if it is real we want to get rid of it because it messes up any attempt at perturbation theory in nuclear structure.

One Answer: $V_{\text{low k}}$

In spirit of effective field theory, restrict the energies in our equations with to those in which the nucleon is a sensible degree of freedom. Replace Schrödinger equation in momentum space:

$$\frac{\hbar^2 k^2}{m_N}\langle\mathbf{k}|\Psi\rangle + \int_{|\mathbf{k}'|=0}^{\infty} d^3k' \; \langle\mathbf{k}|V_{NN}|\mathbf{k}'\rangle\langle\mathbf{k}'|\Psi\rangle = E\langle\mathbf{k}|\Psi\rangle$$

with

$$\frac{\hbar^2 k^2}{m_N}\langle\mathbf{k}|\Psi\rangle + \int_{|\mathbf{k}'|=0}^{\Lambda} d^3k' \; \langle\mathbf{k}|V_{\text{low k}}|\mathbf{k}'\rangle\langle\mathbf{k}'|\Psi\rangle = E\langle\mathbf{k}|\Psi\rangle \; .$$

Here $\mathbf{k}$ is the relative momentum of the two nucleons and Λ is a low momentum scale often taken to be about 2 fm^{-1}, which corresponds to $E_{\text{lab}} = 350$ MeV for collisions. This cutoff should be fine for nuclear structure calculations because they don't consider excitations higher than that.

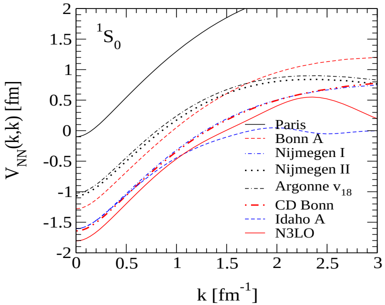
Amazingly...

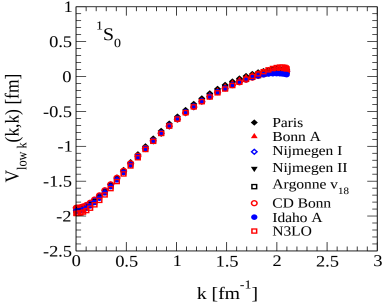
"Low-k-izing" NN Potentials

Doesn't matter which of the very different potentials you start with.

Get a unique $V_{\text{low k}}$!

In coordinate space hard core is gone. Makes certain kind of nuclear-structure calculations much easier, though wth some methods you can still start from the the hard-core potentials.





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Green's Function Monte Carlo

Nearly exact calculations with Argonne v18 up to ^{12}C. Spin and isospin degrees of freedom make Schrödinger equivalent to 270,336 differential equations in 33 variables.

Step 1: Variational Monte Carlo: Minimize

$$E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$

with sophisticated trial variational wave function (schematic here):

$$|\Psi_T\rangle = \left[1 + \sum_{i<j<k} U_{ijk} \right] \left[\mathcal{S} \prod_{i<j} U_{i,j} \right] |\Phi\rangle \ ,$$

where the U's represent two-and three-body correlations and $|\Phi\rangle$ is a Slater determinant.

Green's Function Monte Carolo

Step 2: Green's function Monte Carlo on variational wave function

Propoagate in "imaginary time" τ

$$\begin{aligned} |\Psi(\tau)\rangle &= e^{-(H-E_0)\tau}|\Psi_T\rangle \\ |\Psi_0\rangle &= \lim_{\tau\to\infty} |\Psi(\tau)\rangle \end{aligned}$$

Excited states are damped out as $e^{-(E_n-E_0)\tau}$. Next use

$$e^{-(H-E_0)\tau} = [e^{-(H-E_0)\Delta\tau}]^n$$

and define

$$G(\mathbf{R}',\mathbf{R}) = \langle \mathbf{R}'|e^{-(H-E_0)\Delta\tau}|\mathbf{R}\rangle$$

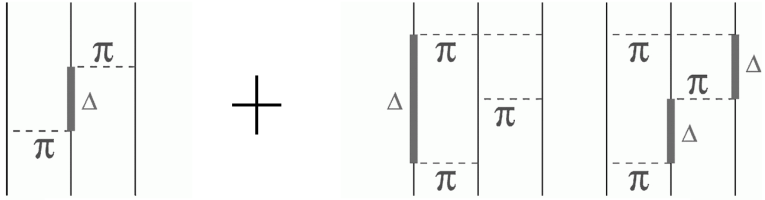
to get

$$\langle \mathbf{R_n}|\Psi(\tau)\rangle = \int G(\mathbf{R_n},\mathbf{R_{n-1}})\cdots G(\mathbf{R_1},\mathbf{R_0})\; d\mathbf{R}_{n-1}\cdots d\mathbf{R}_0 \;,$$

a many-dimensional integral that requires Monte Carlo to evaluate.

Results

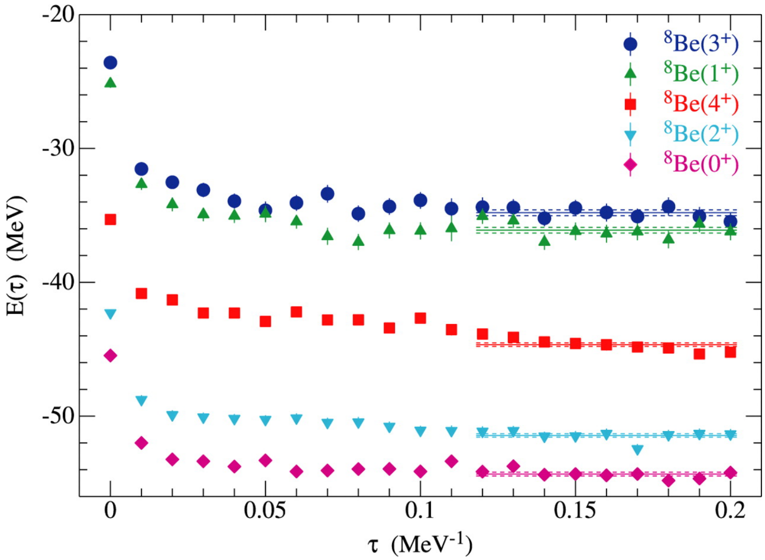
Not good unless v_{ij} supplemented by three-body interaction V_{ijk}:



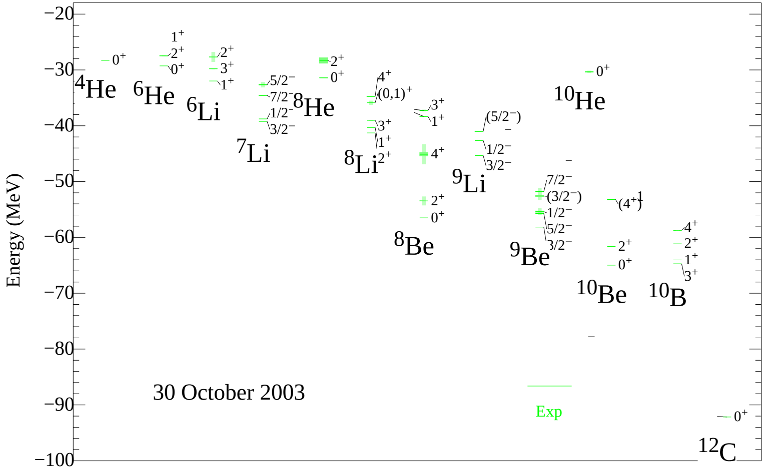
This and most other GFMC pictures from S. C. Pieper and R. B. Wiringa, Annu. Rev. Nucl. Part. Sci. 51, 53 (2001)

- First term most important
- Also a short range piece with 3 or 4 more independent parameters, which are fit to about 20 nuclear levels

Convergence



Spectra



Updated version at, e.g,
http://www.fy.chalmers.se/conferences/inpc2004/Scientific/Programme/Friday/plenary/t4.pdf

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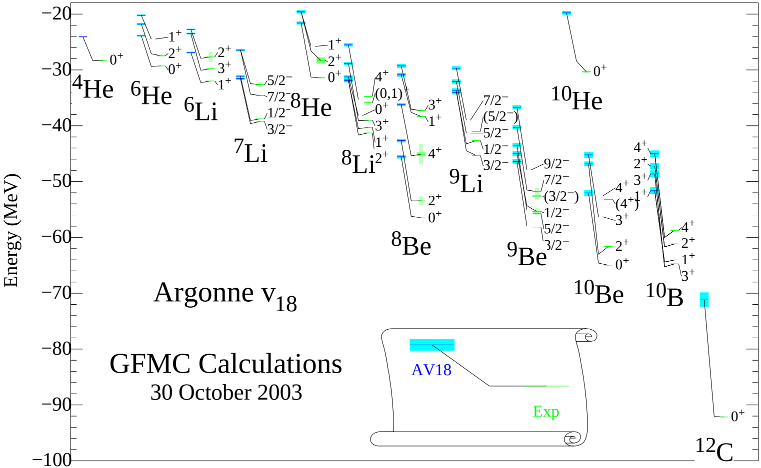

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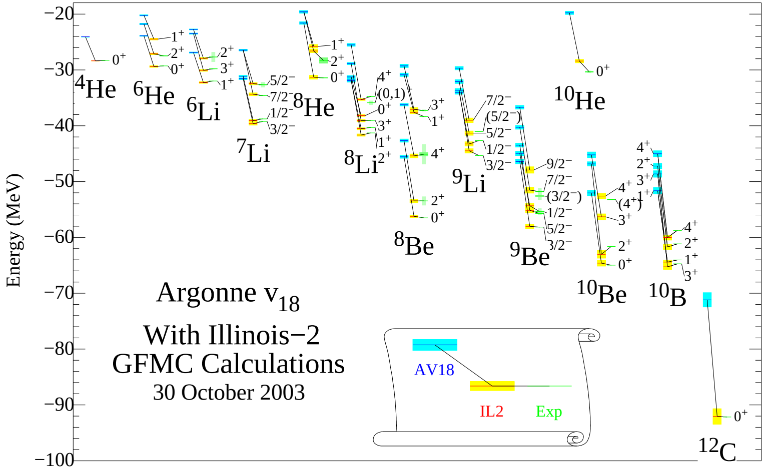

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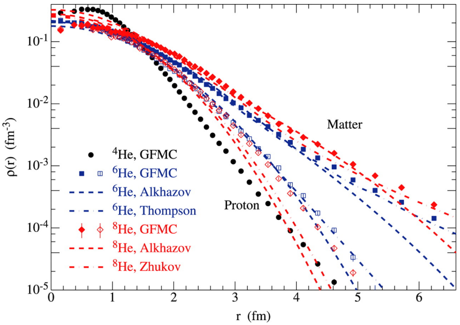
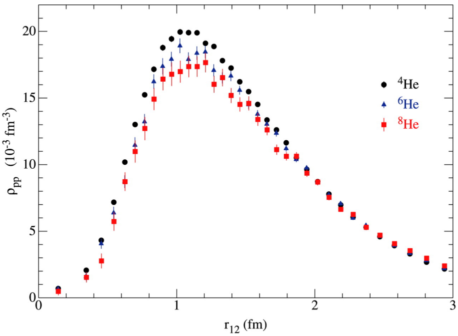
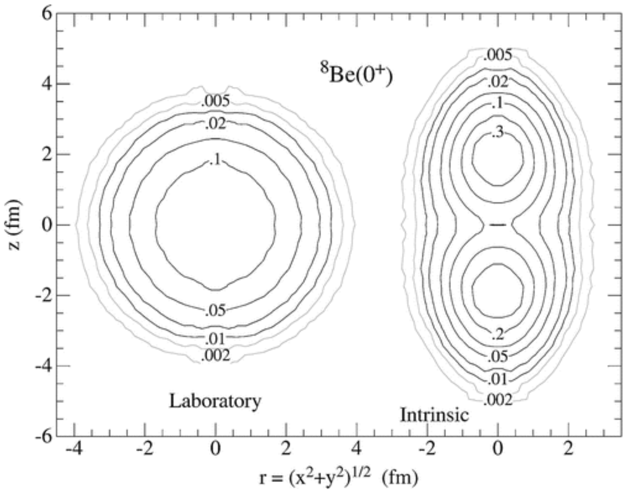
Densities and Correlations





Intrinsic Density!



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Another Approach: No-Core Shell Model

Start with the full Hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

Add an oscillator potential that acts on center of mass

$$V_{CM} = \frac{1}{2} m A \Omega^2 \left(\frac{1}{A} \sum_i \vec{r}_i \right)^2$$

Together these give

$$H_\Omega = \boxed{\sum_i \frac{p_i^2}{2m} + \sum_i \frac{m\Omega^2 r_i^2}{2}} + \boxed{\sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} - \sum_{i<j} \frac{m\Omega^2}{A} (\vec{r}_i - \vec{r}_j)^2}$$

$\Uparrow$ Harmonic Oscillator

$\Uparrow$ "Residual" Part

Basic Idea of Shell Model

H_{CM} doesn't affect intrinsic excitations. Ground state of H_Ω is a product of intrinsic ground state and center-of-mass oscillation. Can get ground-state energy by subtraction $\hbar\Omega$.

Eigenstates of "one-body" oscillator part are localized Slater determinants, the simplest many-body states:

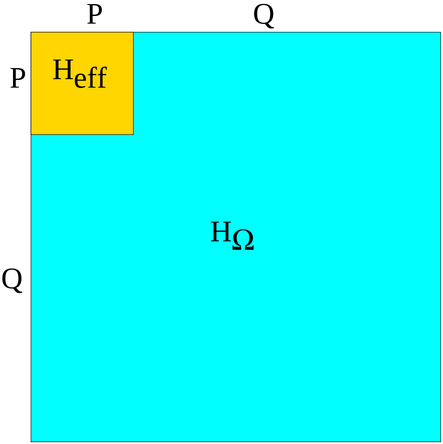
$$\psi(\vec{r}_1 \cdots \vec{r}_n) = \begin{vmatrix} \phi_i(\vec{r}_1) & \phi_j(\vec{r}_1) & \cdots & \phi_l(\vec{r}_1) \\ \phi_i(\vec{r}_2) & \phi_j(\vec{r}_2) & \cdots & \phi_l(\vec{r}_1) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_i(\vec{r}_n) & \phi_j(\vec{r}_n) & \cdots & \phi_l(\vec{r}_n) \end{vmatrix}$$

$$\longrightarrow a_i^\dagger a_j^\dagger \cdots a_l^\dagger |0\rangle$$

in second quantization. They make a convenient basis for diagonalization of H_Ω (the oscillator potential makes them particularly convenient). To get a complete set just put distribute the A particles, one in each oscillator state, in all possible ways.

Truncating the Model Space

Can't include all oscillator levels. Results in a division of Hilbert space for A-body system into P space, which is treated, and Q space, which is not. When constructing Hamiltonian want:



As a result can't use real Hamiltonian. Want to find H_{eff} s.t.

$$\begin{aligned} H_{\Omega}|\Psi_i\rangle &= E_i|\Psi_i\rangle \\ H_{\text{eff}}P|\Psi_i\rangle &= E_iP|\Psi_i\rangle \end{aligned}$$

where the *operator* P projects wave functions onto the P space, and $i = 1, \ldots, \dim(P)$.

Finding the Effective Hamiltonian

Here's the simplest way. Noting that $|\Psi_i\rangle = P|\Psi_i\rangle + Q|\Psi_i\rangle$ and that $P^2 = P$, $Q^2 = Q$, and letting $H = H_\Omega$:

$$PH|\Psi_i\rangle = \boxed{E_i P|\Psi_i\rangle = PHP|\Psi_i\rangle + PHQ|\Psi_i\rangle} \quad (1)$$

$$QH|\Psi_i\rangle = \boxed{E_i Q|\Psi_i\rangle = QHP|\Psi_i\rangle + QHQ|\Psi_i\rangle} \quad (2)$$

Use (2) to solve for $Q|\Psi_i\rangle$ in terms of $P|\Psi_i\rangle$:

$$Q|\Psi_i\rangle = \frac{1}{E_i - QH} QHP|\Psi_i\rangle$$

and plug into (1):

$$E_i P|\Psi_i\rangle = \left[PHP + PH\frac{1}{E_i - QH}QHP\right] P|\Psi_i\rangle$$

so

$$\boxed{H_{\text{eff}} = PHP + PH\frac{1}{E_i - QH}QHP}$$

Finding the Effective Hamiltonian

$H_{\text{eff}} = PHP + PH\frac{1}{E_i - QH}QHP$ is the "Bloch-Horowitz" equation. H_{eff} is energy-dependent, that is it depends on the eivenvalue of the state you're considering, but there are techniques (which, luckily for you, I won't go into) for obtaining an H_{eff} that is not.

The No-Core Approach

1. Diagaonlize $T + v_{ij}$ for two particles in a very large space (levels up to $\approx 50 - 100\hbar\Omega$ so that solutions are essentially exact).
2. Construct two-body H_{eff} (which will look something like $V_{\text{low k}}$) for smaller space ($\approx 20 - 30\hbar\Omega$) and use it together with V_{ijk} for three-body three-body system (^{3}H, ^{3}He). Assumption: **induced** three-body interactions in a space this size are negligible.
3. Use result to construct new H_{eff} (which is now three-body) in even smaller space ($\approx 10 - 20\hbar\Omega$) and solve diagonalize four-particle system.

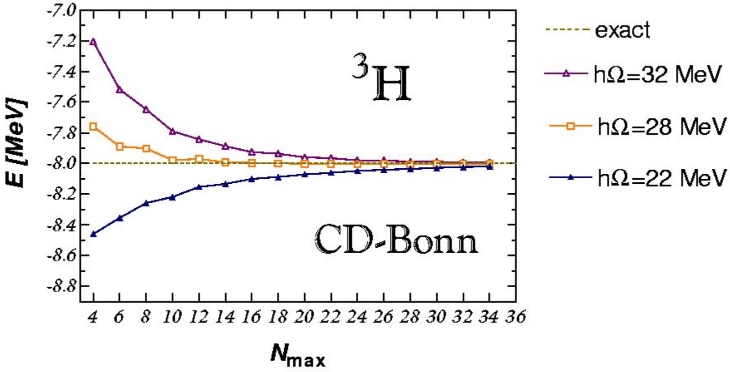
$$\vdots$$

(though you usually assume a three-body H_{eff} is enough).

Results

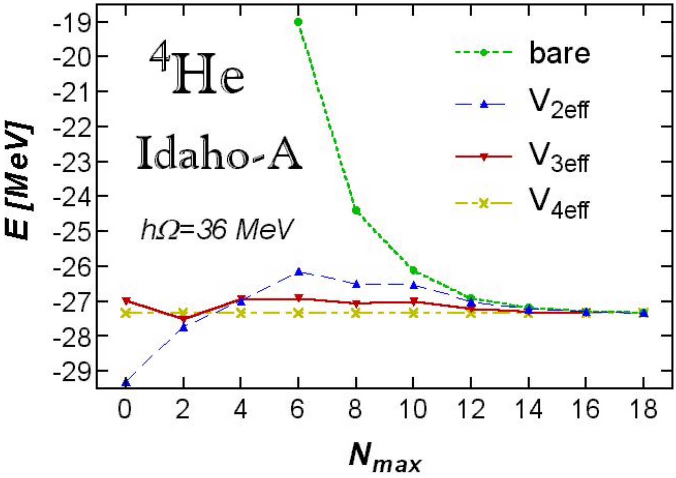
Convergence rate with number of levels depends on the strength Ω of the oscillator potential.

From E. Ormand, http://www.phy.ornl.gov/npss03/ormand2.ppt



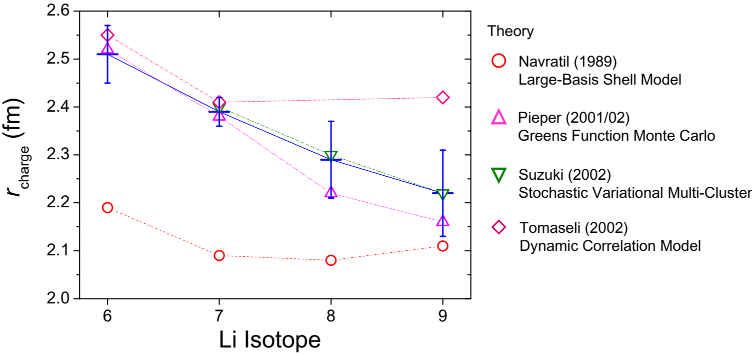
Results

From E. Ormand, http://www.phy.ornl.gov/npss03/ormand2.ppt



Not So Good With All Observables. . .

Harmonic oscillator potential makes asymptotics a bit unrealistic in weakly bound nuclei.



W. Nörtershäuser et al., http://www.edpsciences.org/articles/epja/pdf/first/10050_2005_Article_506053.pdf

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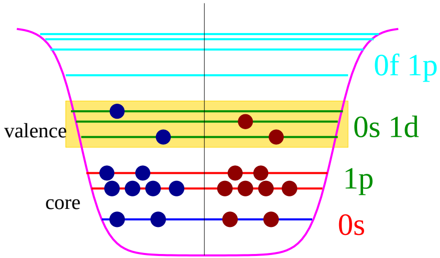
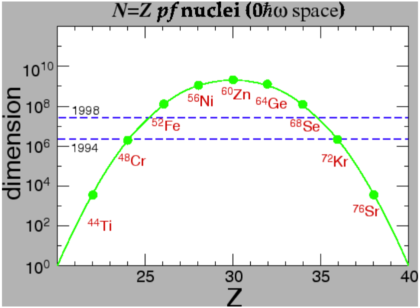
The Regular (Cum Core) Shell Model

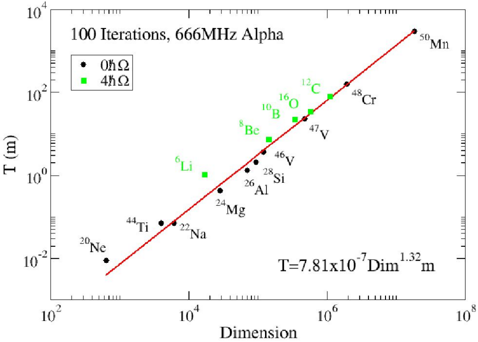
- Core is inert; particles can't move out.
- Particles outside core confined to limited set of valence shells.
- Problem of constructing an effective interaction is complicated by the core. Bootstrapping doesn't work any more. Only half-way decent approach is perturbative expansion of Bloch-Horowitz equation, which is not always convergent. Some phenomenolgy (fitting) is therefore essential.

Example: ^{20}Ne



What the Shell Model Can Handle



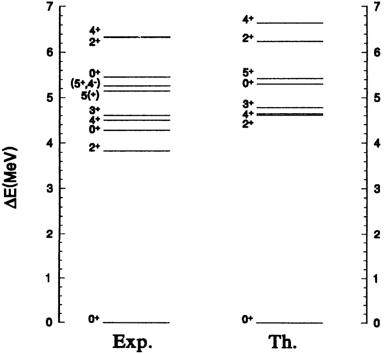


From W. Nazarewicz, http://www-highspin.phys.utk.edu/~witek/

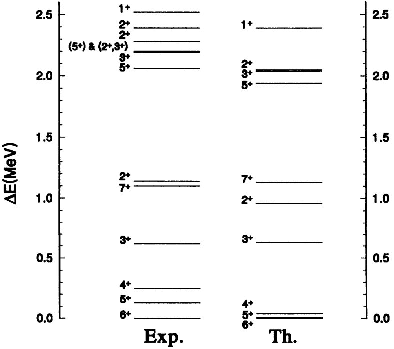
And the problem of constructing an effective interaction gets harder the larger the valence space.

Level of Accuracy (When Good)

^{48}Ca



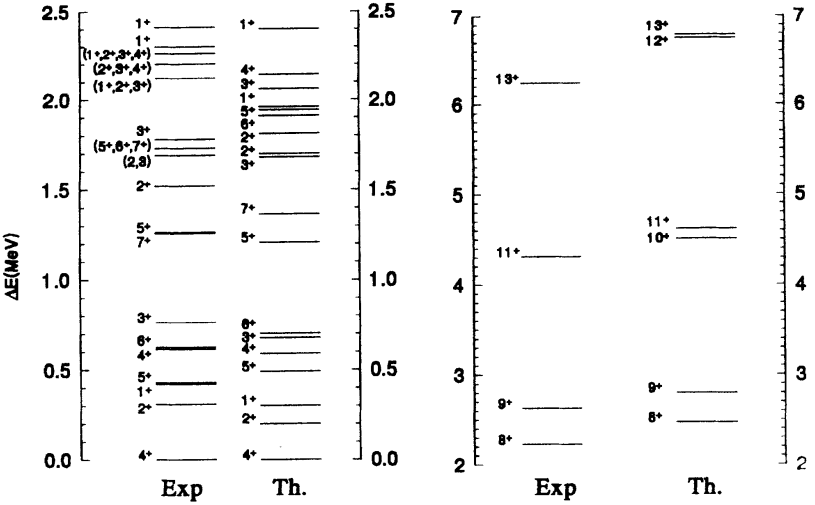
^{48}Sc



This slide and next from A. Poves, J. Phys. G: Nucl. Part. Phys. 25 (1999) 589 597.

Level of Accuracy (When Good)

^{48}V



Next. . .

What To Do in Heavier Nuclei