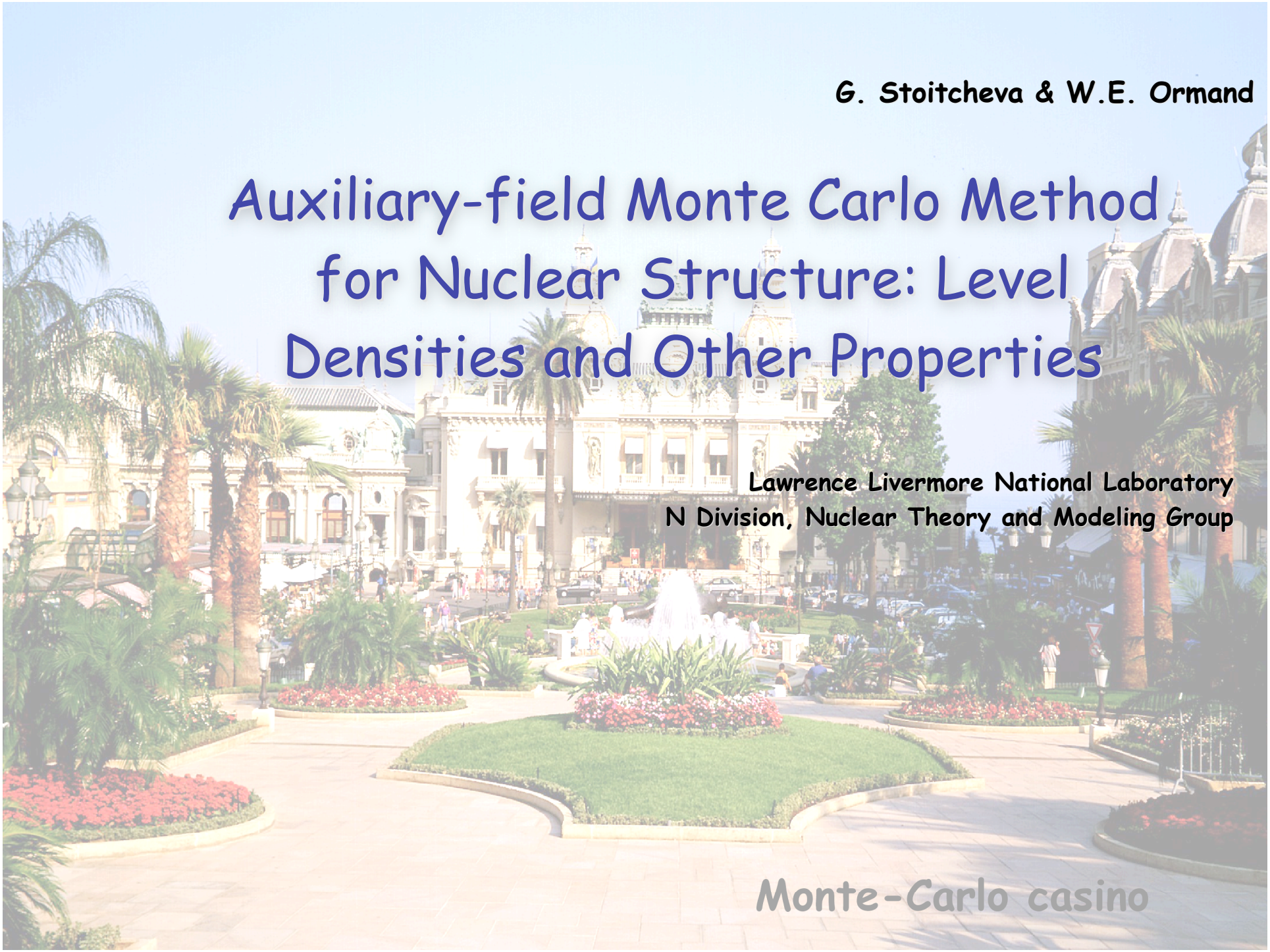
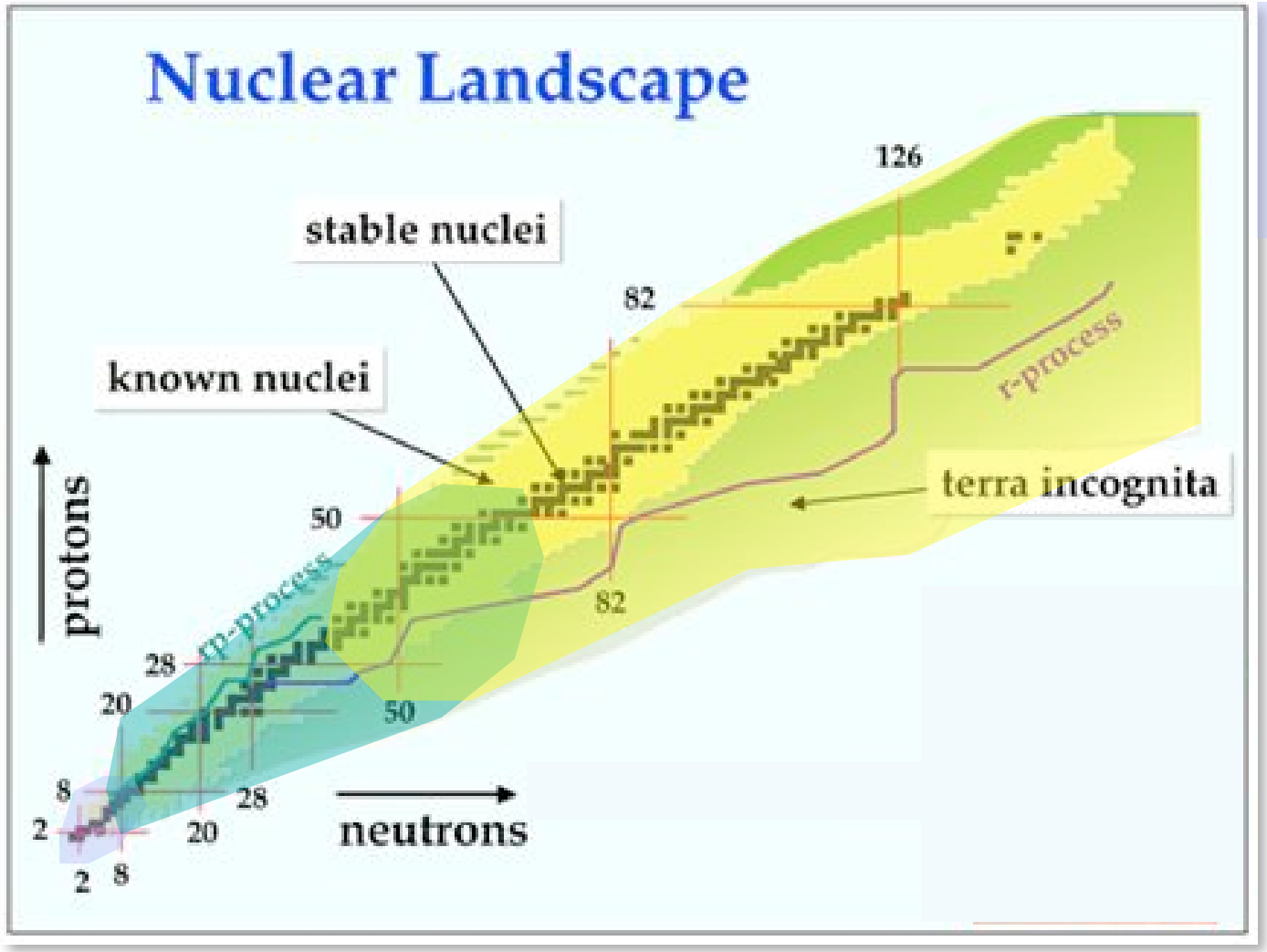
G. Stoitcheva & W.E. Ormand

Auxiliary-field Monte Carlo Method for Nuclear Structure: Level Densities and Other Properties

Lawrence Livermore National Laboratory
N Division, Nuclear Theory and Modeling Group



Generalized Theory for Nuclear Structure

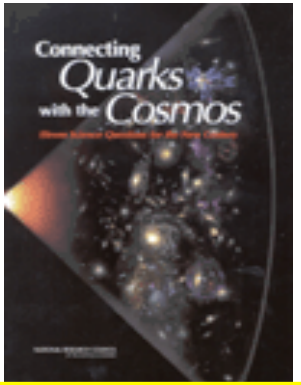


Ab-initio

Quantum Monte Carlo
Symplectic Ab-initio
Coupled-Cluster Techniques

Configuration interaction

Density Functional Theory



Question 3
How were the elements
from
iron to uranium made ?

Research goal

Unified microscopic and predictive theory of all nuclei and their low-energy reactions

Unified: Theoretical approaches overlap and need to be bridged

Microscopic description: Toward derivation of a universal Hamiltonian by combining self-consistent mean-field theory and quantum correlations

All nuclei: To describe the properties of "nuclei" ranging from the deuteron to neutron star

Motivation: Opportunities for the AFMC and Their Impact on Nuclear Structure Studies

We would like to have a theory capable of

Detailed microscopic description of heavy nuclei with realistic effective interactions:

- accurate binding energies to define the limits of stability
- nuclear level densities (Hauser-Feshbach calculations)
- GT response functions (electron-capture rates)
- strength functions (neutron-induced reactions, astrophysics)

Towards developing a tool that will significantly enhance nuclear structure studies

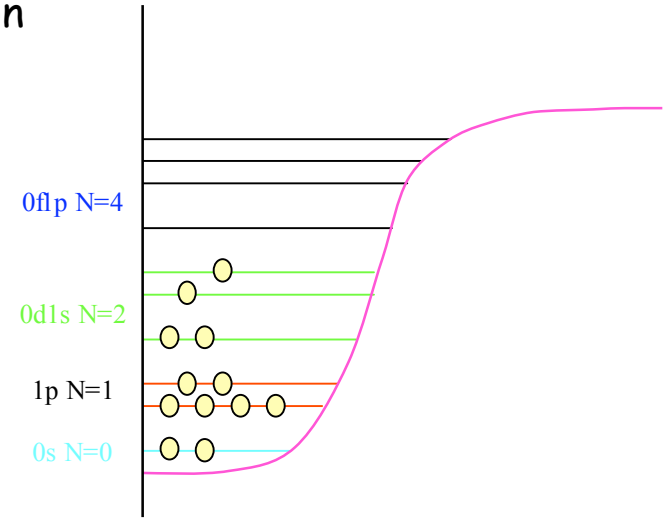
Configuration Interaction

Always the choice of nuclear structure studies (capacity to describe the nuclear dynamics either of single particle or collective nature):

- ✓ Full microscopic accounting of the residual interaction
- ✓ Make many-body wave functions to expand full solution

$$\Phi_i = \sum_n C_{in}\phi_n$$

$$\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1N} \\ H_{21} & H_{22} & & \\ \vdots & & \ddots & \\ H_{N1} & & \cdots & H_{NN} \end{pmatrix} \longrightarrow$$

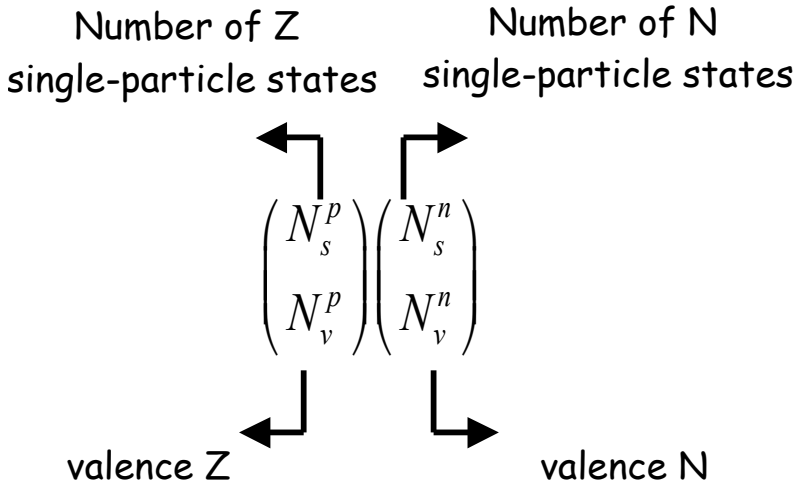


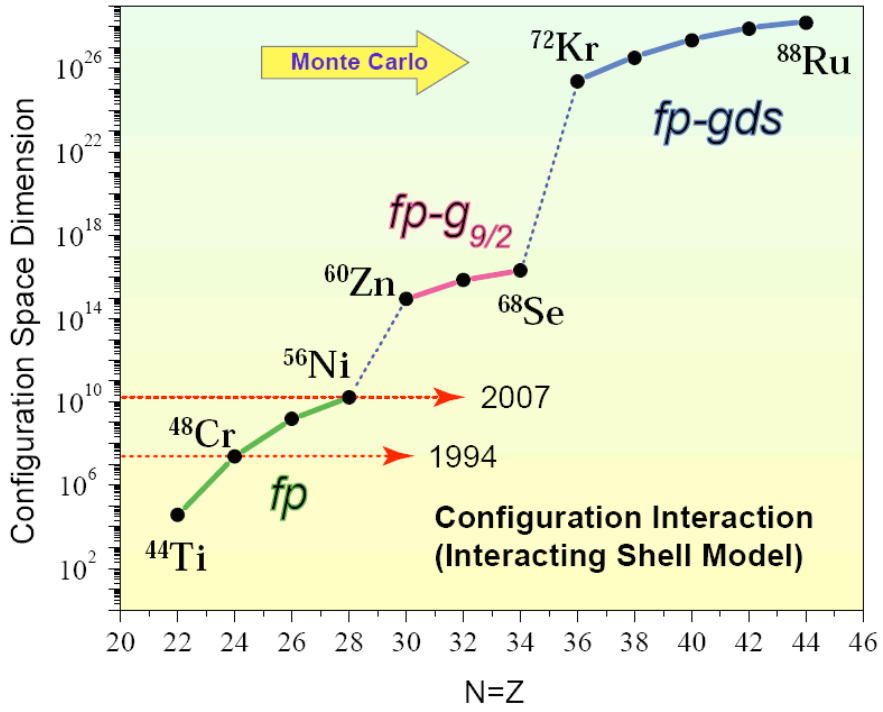
diagonaize the matrix $H_{ij}=\langle\phi_j|H|\phi_i\rangle$ in the basis to obtain eigenvalues

The conventional shell model with a full major shell has been successful up to A~70 due to large dimensions

Challenges

✓ The total number of Slater determinants within a Hilbert space:





Computational limit to 10^{10}

Current nuclear models are inadequate!

Computational scope with traditional methods beyond the capability of any computer.

✓ In the neutron rich side: two contiguous major shells have to be included in the valence space, the Fock space representation

Defeating the Combinatorial Explosion

Have to do something else…. (Steve Koonin, early 1990)

$$E_{GS} = \lim_{\beta\to\infty} \frac{\langle \varphi_0 | e^{-\beta\hat{H}/2} \hat{H} e^{-\beta\hat{H}/2} | \varphi_0 \rangle}{\langle \varphi_0 | e^{-\beta\hat{H}} | \varphi_0 \rangle} = \frac{\langle \varphi_{gs} | \hat{H} | \varphi_{gs} \rangle}{\langle \varphi_{gs} | \varphi_{gs} \rangle}$$

$$E(\beta) = \frac{Tr\left[\hat{H} e^{-\beta\hat{H}}\right]}{Tr\left[e^{-\beta\hat{H}}\right]} \qquad \beta = 1/T$$

The Hamiltonian:

$$H = \sum_\alpha \varepsilon_\alpha \hat{O}_\alpha + \frac{1}{2}\sum_\alpha \lambda_\alpha \hat{O}_\alpha^2$$

Single-particle energy

Density operator

Strength of the TB int.

General Strategy

1. Gaussian (HS) Transformation

$$\int d\sigma e^{-\frac{1}{2}\beta\lambda\left(\hat{O}-s\sigma\right)^2} = \sqrt{\frac{2\pi}{\beta|\lambda|}} \qquad s = \begin{cases} \pm 1 & \text{if } \lambda \le 0 \\ \pm i & \text{if } \lambda > 0 \end{cases}$$

$$e^{-\beta H} = \sqrt{\frac{\beta|\lambda_\alpha|}{2\pi}} \int d\sigma_\alpha e^{-\beta|\lambda_\alpha|\sigma_\alpha^2 + 2\beta(\varepsilon_\alpha + s\sigma_\alpha\lambda_\alpha)\hat{O}_\alpha}$$

One-body operator

Gaussian factor

One-body Hamiltonian

$$\hat{H} \to \hat{h}(\sigma) = \sum_\alpha \left(\varepsilon_\alpha + s_\alpha\lambda_\alpha\sigma_\alpha\right)\hat{O}_\alpha$$

auxiliary-fields

2. Break up the imaginary time-evolution operator into time slices

$$e^{-\beta\hat{H}} = \left(e^{-\Delta\beta\hat{H}}\right)^{N_t} = \underbrace{e^{-\Delta\beta\hat{H}} \cdots e^{-\Delta\beta\hat{H}}}_{N_t} \qquad \Delta\beta = \beta/N_t$$

3. Any observable can be defined as

$$\left\langle \hat{O} \right\rangle = \frac{\int \prod_{\alpha,n} d\sigma_{\alpha,n} e^{-\frac{\Delta\beta}{2}\sum_{\alpha}|\lambda_\alpha|\sigma^2{}_\alpha} Tr\left[e^{-\Delta\beta\hat{h}(\sigma_1)}\cdots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right] \frac{Tr\left[\hat{O}e^{-\Delta\beta\hat{h}(\sigma_1)}\cdots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]}{Tr\left[e^{-\Delta\beta\hat{h}(\sigma_1)}\cdots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]}}{\int \prod_{\alpha,n} d\sigma_{\alpha,n} e^{-\frac{\Delta\beta}{2}\sum_{\alpha}|\lambda_\alpha|\sigma^2{}_\alpha} Tr\left[e^{-\Delta\beta\hat{h}(\sigma_1)}\cdots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]}$$

$$= \frac{\int \prod_{\alpha,n} d\sigma_{\alpha,n} W(\sigma) \langle O \rangle_\sigma}{\int \prod_{\alpha,n} d\sigma_{\alpha,n} W(\sigma)}$$

The dimension of the integral is $N^2{}_s N_t$

10^{22} states = $2*10^5$ fields

But W(s) must be positive

The weight function:

$$W(\sigma) = e^{-\frac{\Delta\beta}{2}\sum_{\alpha}|\lambda_\alpha|\sigma_\alpha^2} Tr\left[e^{-\Delta\beta\hat{h}(\sigma_1)}\cdots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]$$

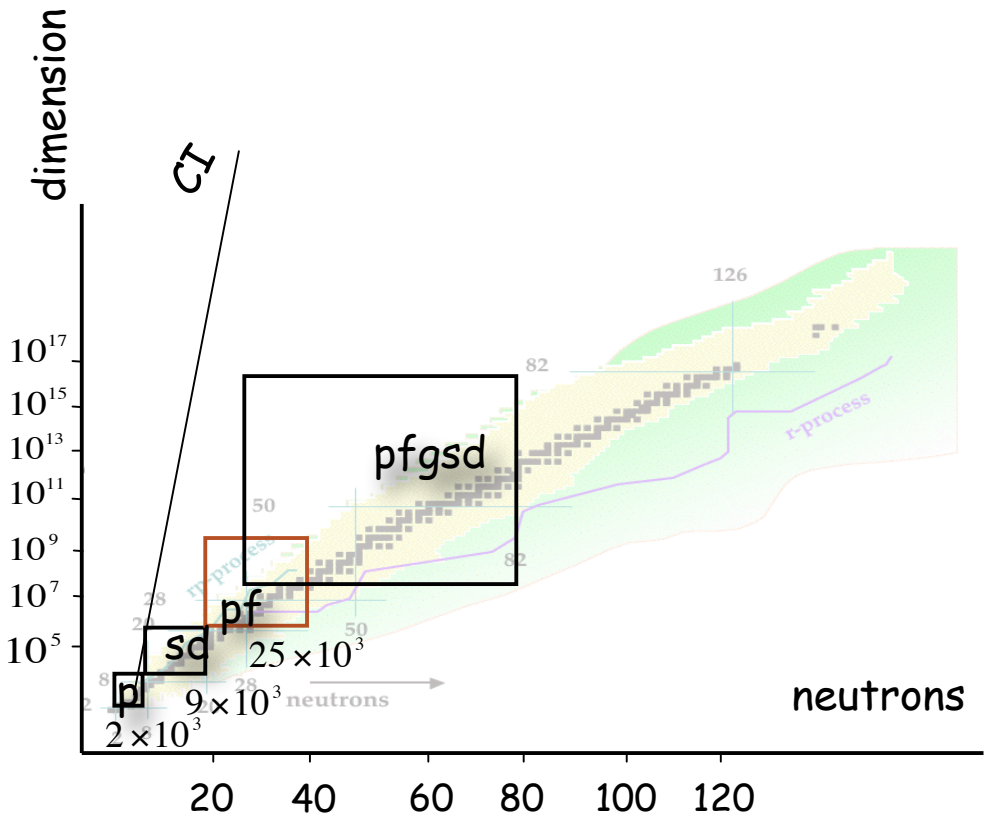
$$\left\langle \hat{O} \right\rangle_{\mathrm{MC}} = \frac{\sum_k \left\langle \hat{O} \right\rangle_{\sigma_k} W(\sigma_k)/|W(\sigma_k)|}{\sum_k W(\sigma_k)/|W(\sigma_k)|}$$

The sign of the MC weight function

The Power of AFMC

✓ AFMC is a statistical approach within the shell-model framework which can provide exact results for systems with extraordinarily large dimensions (10^{21} and beyond)

✓ AFMC is ideally suited for parallel, high-performance computing



The "catch" in AFMC

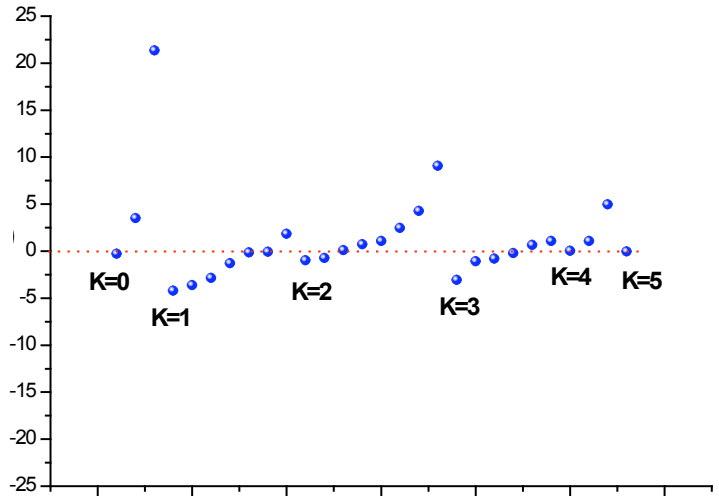
We need to have W(σ) to be positive definite!

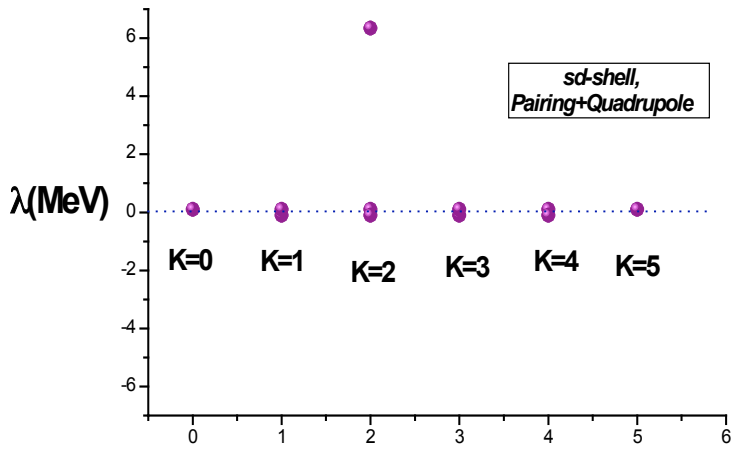
$$\langle \hat{O} \rangle = \frac{\int |W(\sigma)| \langle \hat{O} \rangle_\sigma W(\sigma)/|W(\sigma)|}{\int |W(\sigma)| W(\sigma)/|W(\sigma)|} \quad \rightarrow \quad \langle \hat{O} \rangle_{\mathrm{MC}} = \frac{\sum_k \langle \hat{O} \rangle_{\sigma_k} W(\sigma_k)/|W(\sigma_k)|}{\sum_k W(\sigma_k)/|W(\sigma_k)|}$$

Our two-body Hamiltonian: $H_2 = \frac{1}{2} \sum_{K,M} (-)^M E_\pi^K \rho^{K,M} \rho^{K,-M}$

The time-reversal properties play a central role

Lang's rule for a "good" interaction: $(-1)^K \pi_\alpha \lambda_\alpha < 0$ (attractive)

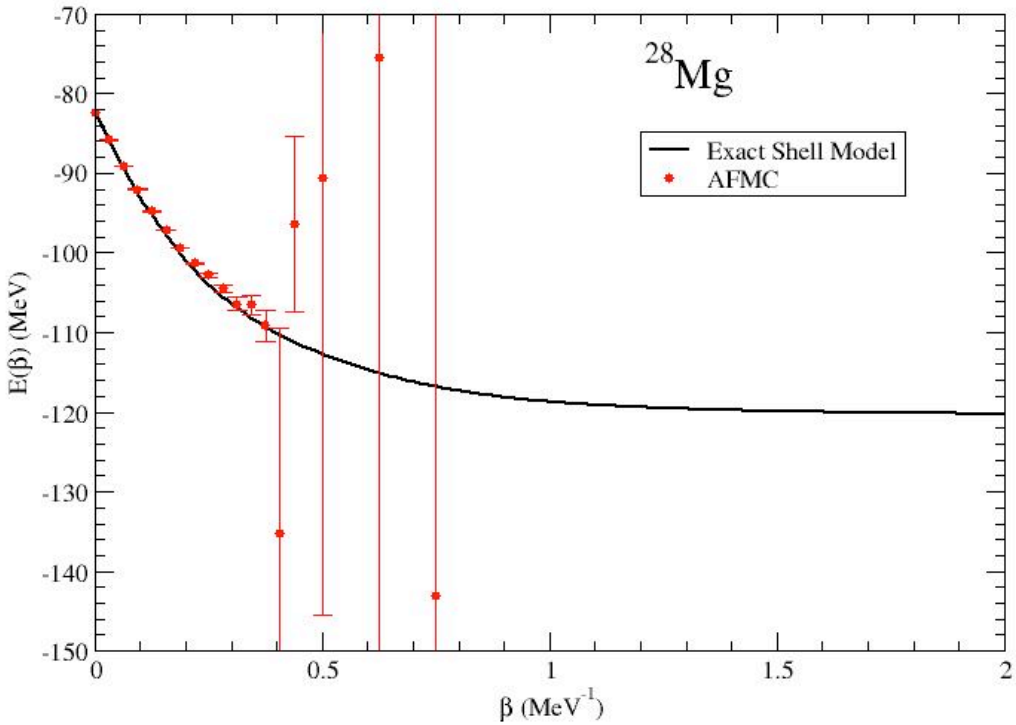




(Lang at. al, PRC, 1993)

Auxiliary-field Monte Carlo Method

$$\langle \hat{O} \rangle = \frac{\int |W(\sigma)| \langle \hat{O} \rangle_\sigma \, W(\sigma)/|W(\sigma)|}{\int |W(\sigma)| W(\sigma)/|W(\sigma)|} \quad \rightarrow \quad \langle \hat{O} \rangle_{\mathrm{MC}} = \frac{\sum_k \langle \hat{O} \rangle_{\sigma_k} W(\sigma_k)/|W(\sigma_k)|}{\sum_k W(\sigma_k)/|W(\sigma_k)|}$$



AFMC before: Useless with realistic interactions

Interdisciplinary Interest in the Fermionic Sign Problem

Physics Now

Reviews
by leading physicists in the
International Union of Pure and Applied Physics

Editor
Jon Ogborn

We also note that there are important problems that are not solved - both molecular dynamics and Monte Carlo methods in their original forms deal with classical statistical mechanics, and though there exist some extensions to deal with quantum statistical mechanics, there are sometimes severe difficulties, such as the famous "minus sign problem" encountered when one tries to extend the quantum Monte Carlo methods to fermionic degrees of freedom. If a breakthrough in this area could be found, this numerical approach to statistical mechanics would find widespread application to condensed matter systems at low temperature (e.g. magnetism, superconductors, semiconductors, metal-insulator transitions).

Matthias Troyer, Uwe-Jens Wiese, Computational complexity and fundamental limitations to fermionic quantum Monte Carlo simulations, PRL 94 (2005)

Congjun Wu, Shou-Cheng Zhang, A sufficient condition for the absence of the sign problem in the fermionic quantum Monte-Carlo algorithm, Phys. Rev. B 71 (2005)

Henelius, P. and A. W. Sandvik: Sign problem in Monte Carlo simulations of frustrated quantum spin systems. Phys. Rev. B 62 (2000)

Chris Adami and Steven E. Koonin, Complex Langevin Equation and the Many-Fermion Problem (2000)

Yoshihiro Asai: Adaptive Sampling Approach to the negative sign-problem in the Auxiliary Field Quantum Monte Carlo, (1998)

T.D. Kieu and C.J. Grifin: Tackling the sign problem, (1993)

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Defeating the Sign Problem: Shifted-Contour Method for AFMC

$$\hat{H} = \sum_\alpha \varepsilon_\alpha \hat{O}_\alpha + \frac{1}{2}\sum_\alpha \lambda_\alpha \hat{O}_\alpha^2$$

Mean-field density

$$\hat{O}_\alpha \to \hat{O}_\alpha - \langle \hat{O}_\alpha \rangle$$

Shift the one-body operator

$$\hat{H} = \sum_\alpha \varepsilon_\alpha \hat{O}_\alpha + \frac{1}{2}\sum_\alpha \lambda_\alpha \left(\hat{O}_\alpha - \langle \hat{O}_\alpha \rangle\right)^2 + \frac{1}{2}\sum_\alpha \lambda_\alpha \left(2\langle \hat{O}_\alpha \rangle \hat{O}_\alpha - \langle \hat{O}_\alpha \rangle^2\right)$$

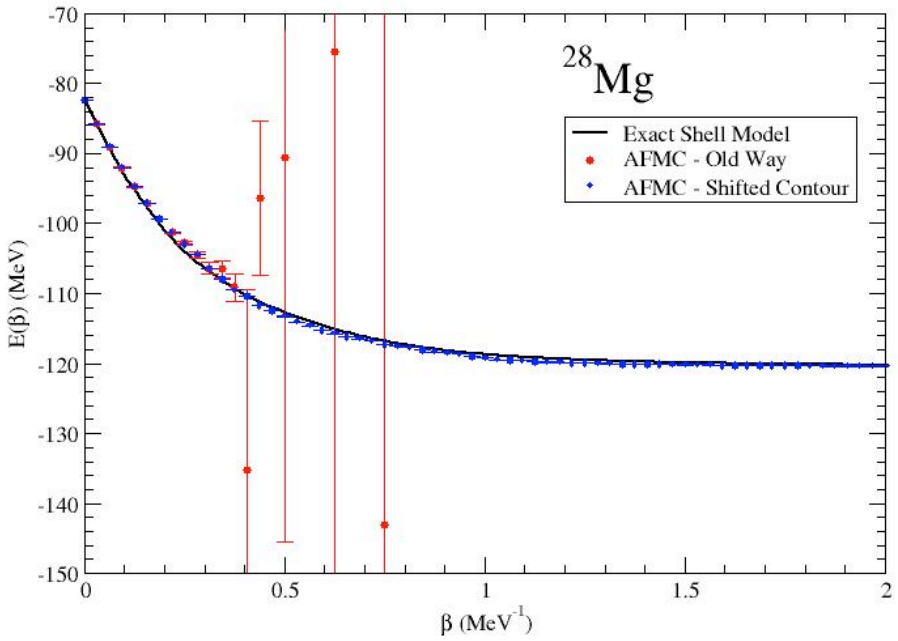
Our two-body Hamiltonian does not change!

⇓

This shifts each auxiliary field by $\langle \hat{O}_\alpha \rangle$ with the net effect of suppressing the sign problem

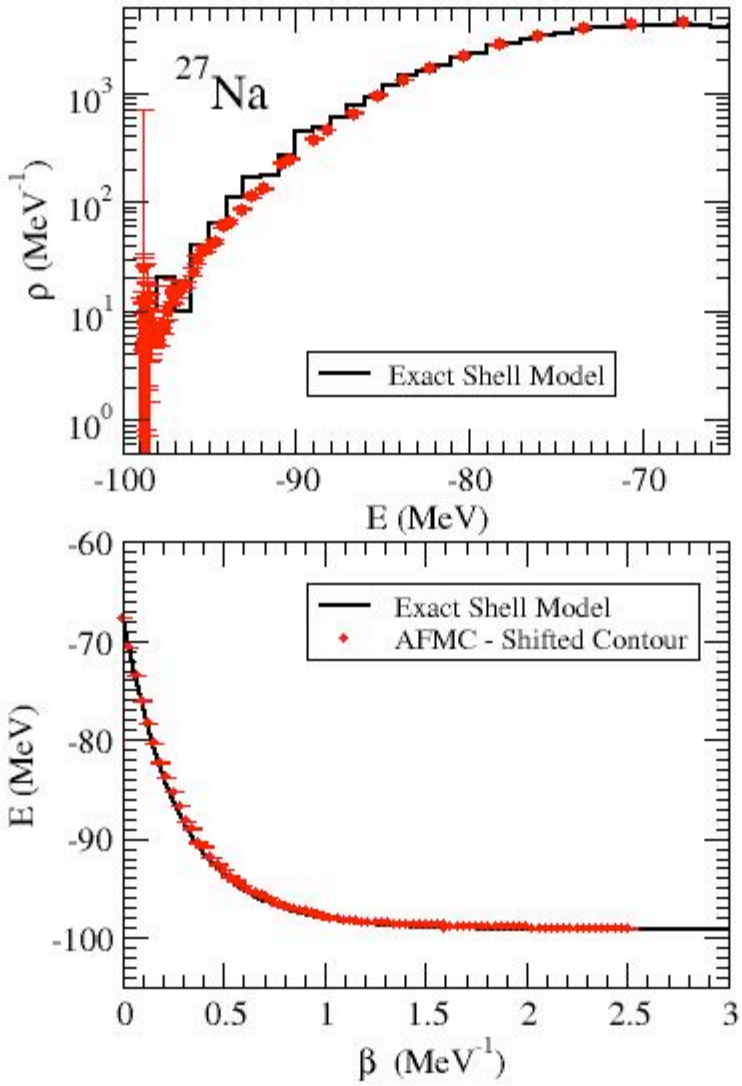
$$e^{-\beta H} = \sqrt{\frac{|\lambda_\alpha|}{2\pi}} \int d\sigma_\alpha e^{-\frac{1}{2}|\lambda_\alpha|\sigma_\alpha{}^2 - \lambda_\alpha\left(2 s_\alpha \sigma_\alpha \langle \hat{O}_\alpha \rangle + \langle \hat{O}_\alpha \rangle\right) - \Delta\beta h(\sigma)}$$

Realistic resolution within AFMC



AFMC now: First successful results

We Defeated the Sign Problem



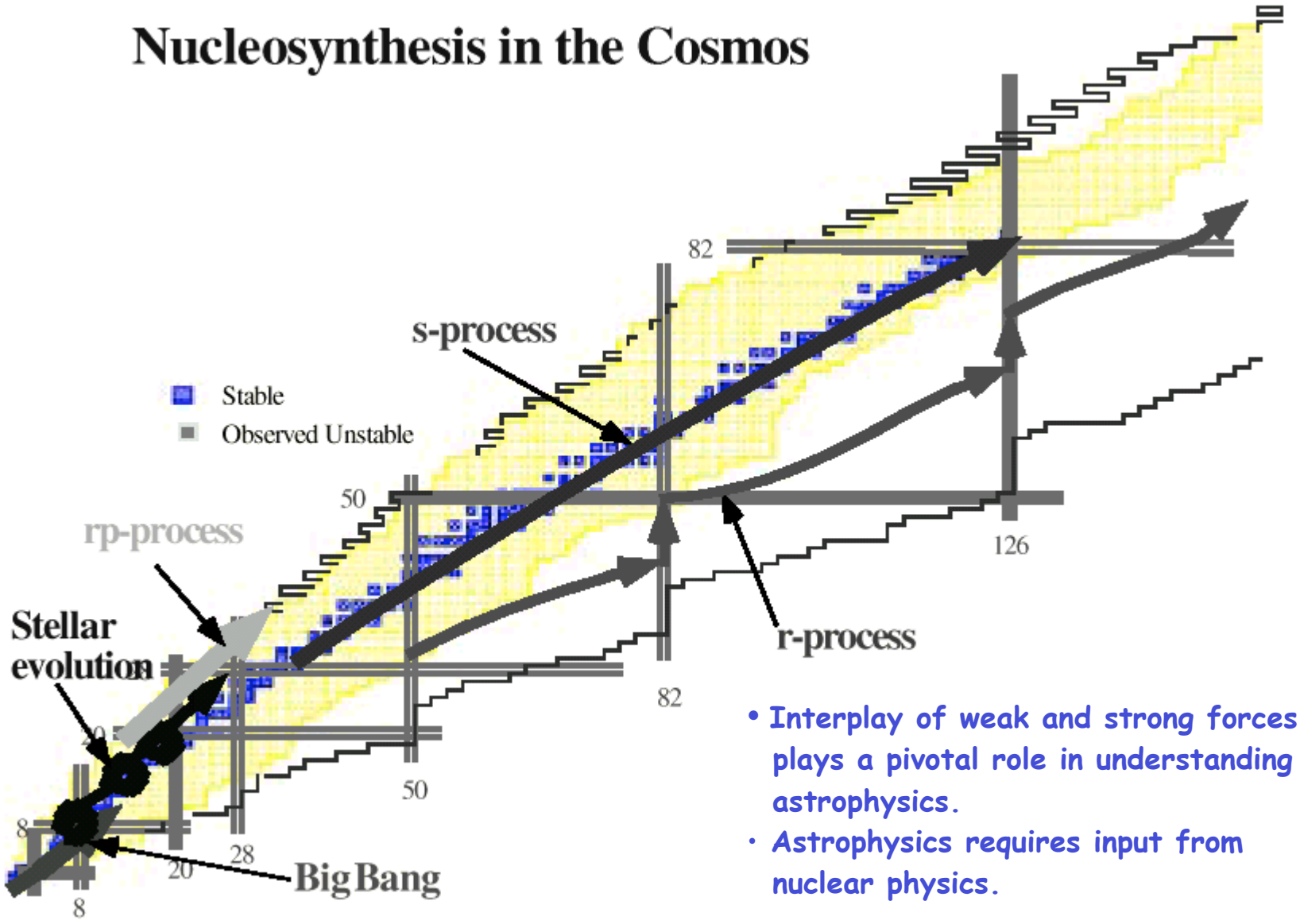
We can calculate level densities:

$$\rho(E) = \frac{e^{\ln Z + \beta E}}{\sqrt{-\frac{2\pi}{\beta}\frac{dE}{d\beta}}}$$

$$\ln Z(\beta) = \ln Z(0) - \int_0^\beta d\beta' E(\beta')$$

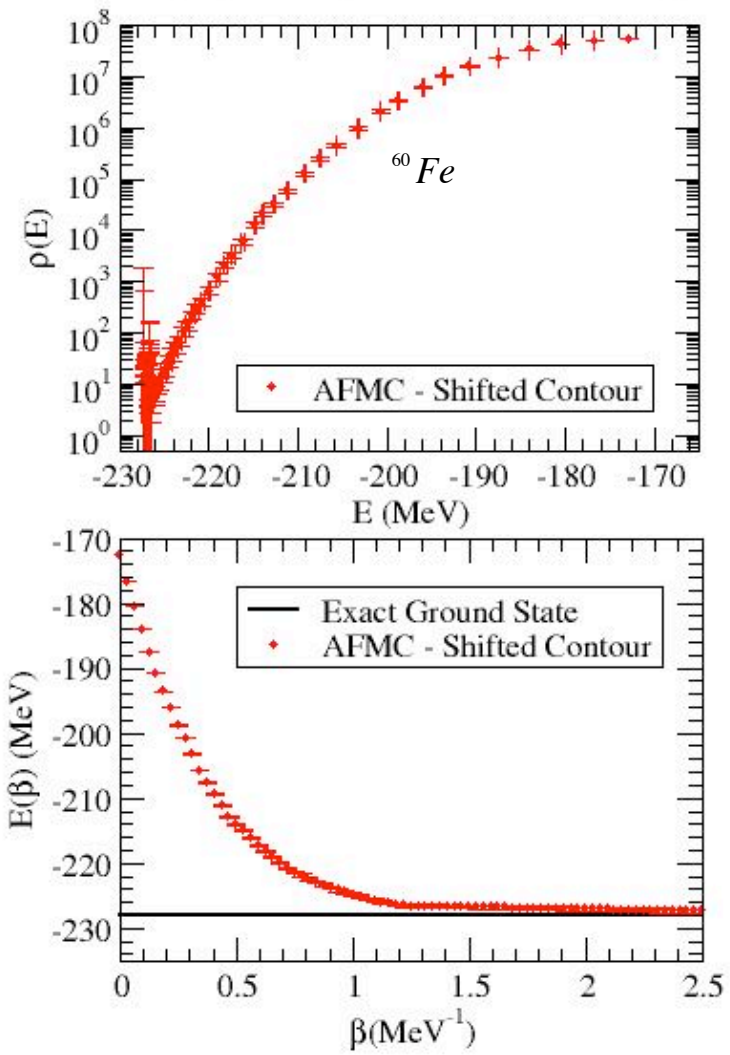
First result ever for an odd nucleus!
We verified that we can
solve the problem exactly

Scientific triple point:
nuclear structure, nuclear astrophysics, weak interactions



- Interplay of weak and strong forces plays a pivotal role in understanding astrophysics.
- Astrophysics requires input from nuclear physics.

Probing Heavier Nuclei



More…

Truly detailed analysis of intermediate-mass nuclei at the limit of stability:

Binding energies

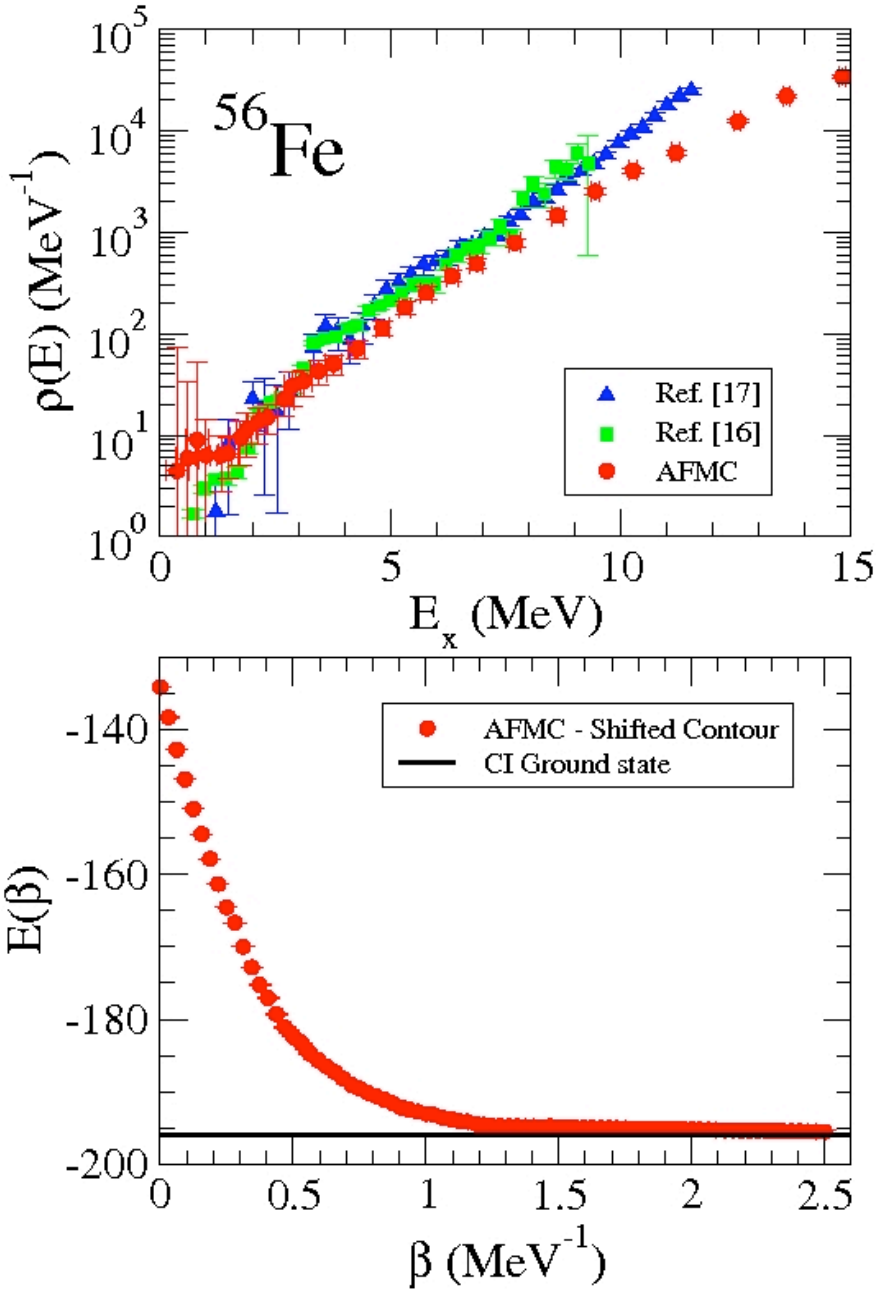
Strength functions

Weak transition rates

Even and Odd nuclei

We offer a method that can revolutionize Nuclear Structure

Jz = 0 is ≈ 501M



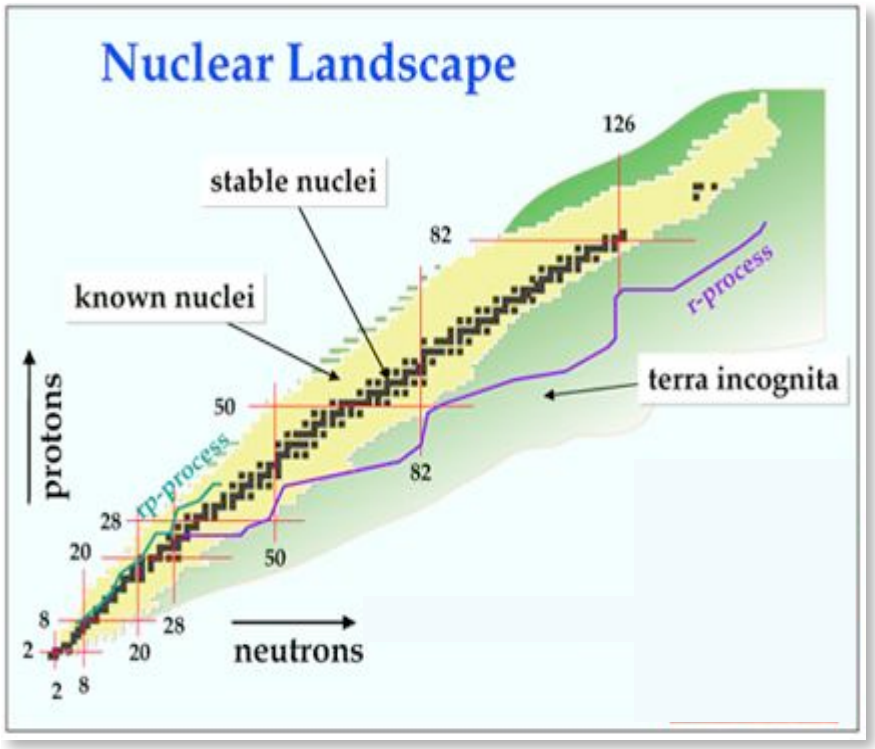
[17] A. Schiller et al., Phys. Rev. C 68, 054326 (2003).
[16] A. V. Voinov et al., Phys. Rev. C 74, 014314 (2006).

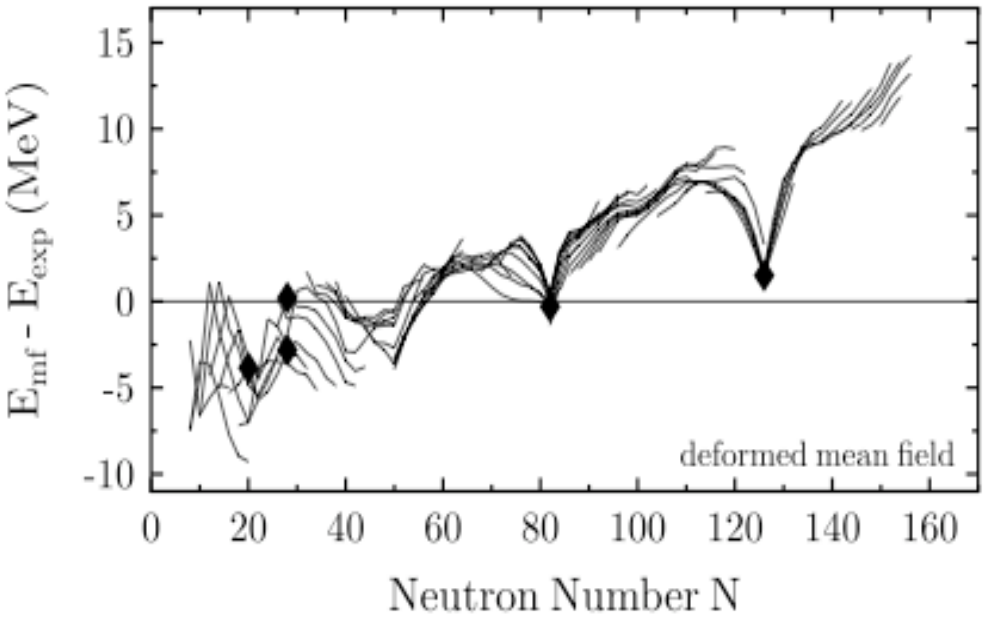
AFMC: -195.687(107) MeV
CI: -195.901MeV

Challenges

Coupled with LLNL supercomputing capability we will deliver the foundation for an entirely new framework to describe the properties of nuclei

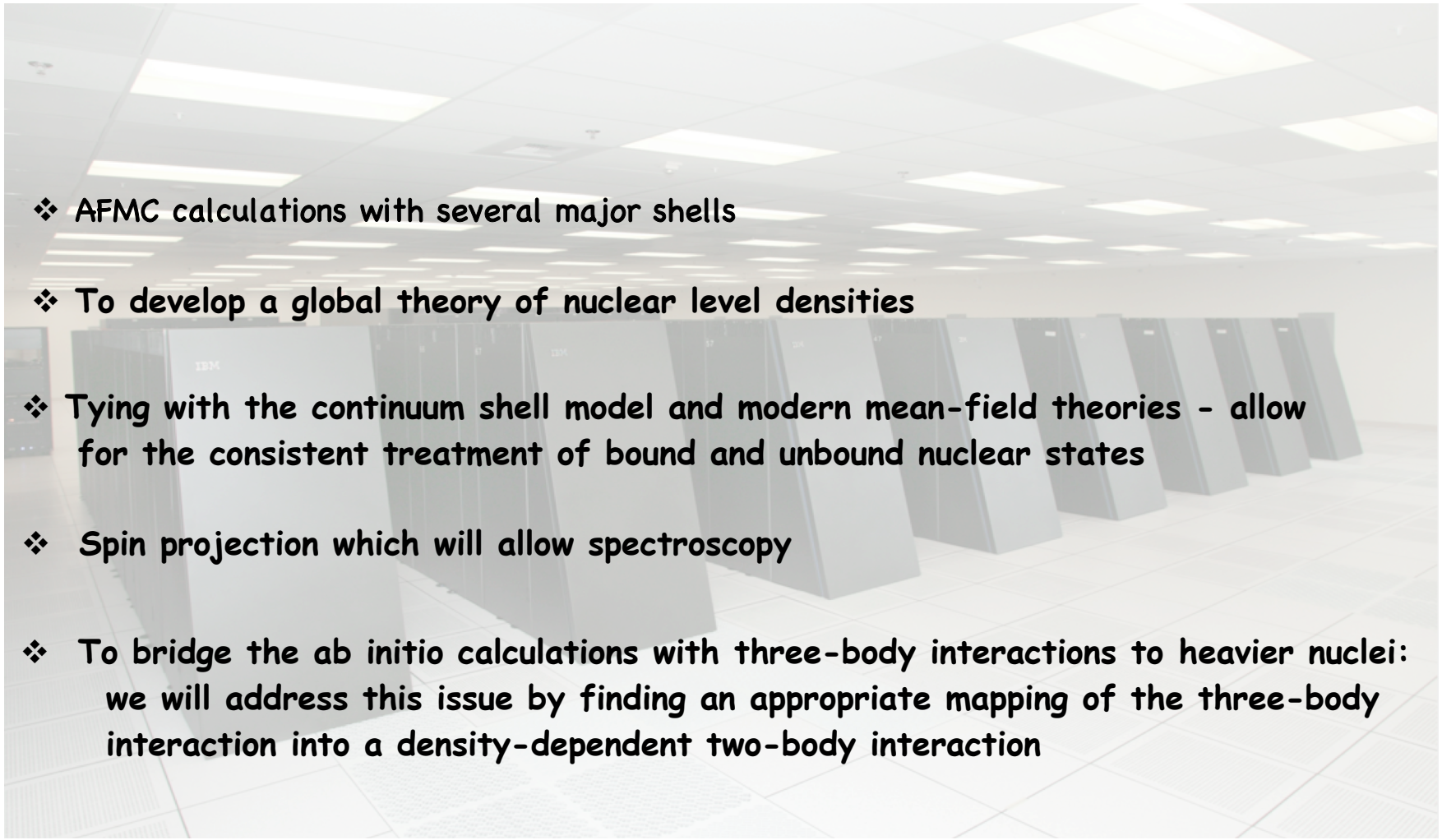
We will combine the AFMC method with Hartree-Fock to develop a universal picture of nuclei that includes the full range quantum effects. All nuclei from $16 \leq A \leq 120$



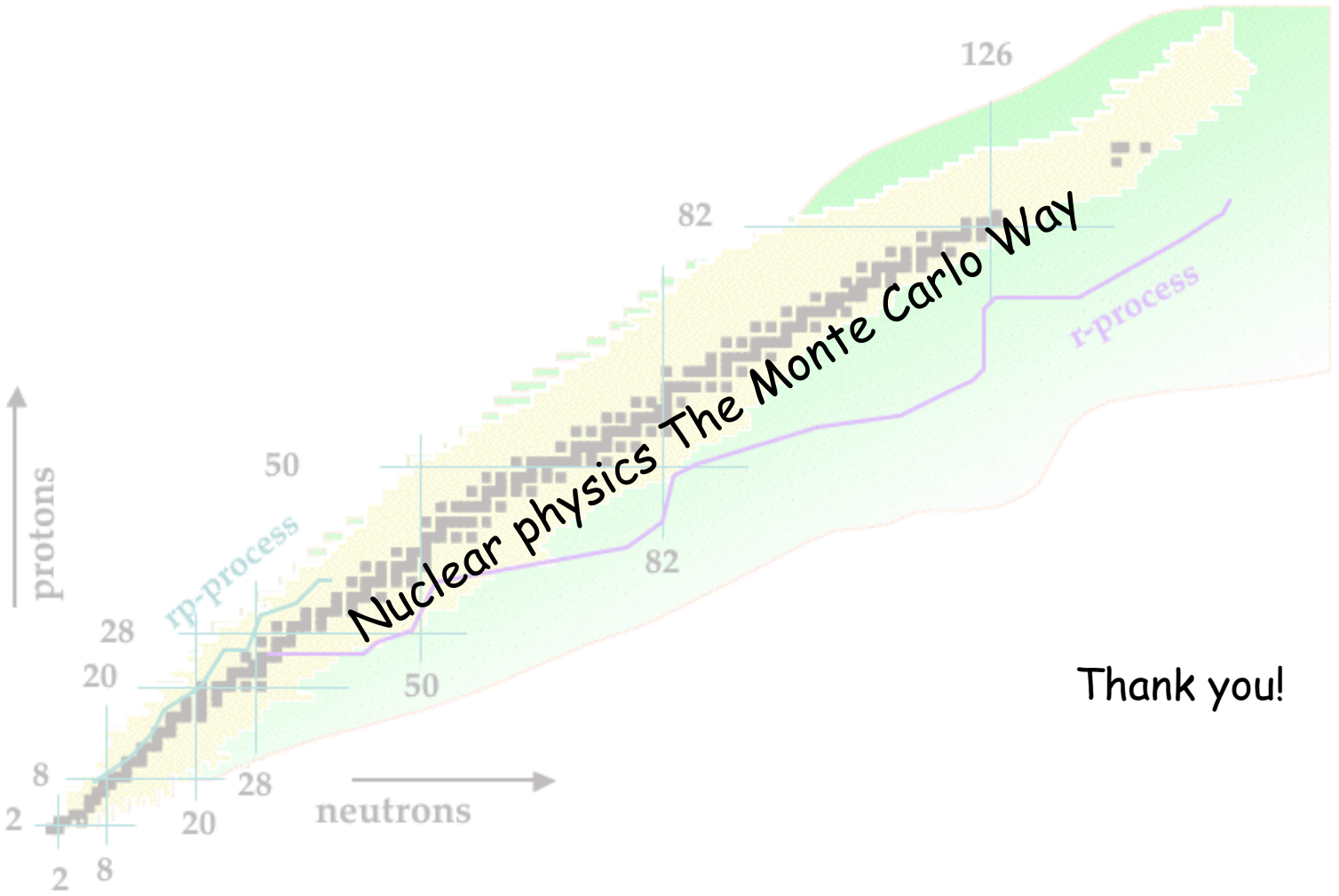


M. Bender, G.F. Bertsch, and P.-H. Heenen, PRC73 034322 (2006)

Complimentary…



- AFMC calculations with several major shells
- To develop a global theory of nuclear level densities
- Tying with the continuum shell model and modern mean-field theories - allow for the consistent treatment of bound and unbound nuclear states
- Spin projection which will allow spectroscopy
- To bridge the ab initio calculations with three-body interactions to heavier nuclei: we will address this issue by finding an appropriate mapping of the three-body interaction into a density-dependent two-body interaction



Thank you!

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