Effect of nuclear structure on Type Ia supernova nucleosynthesis

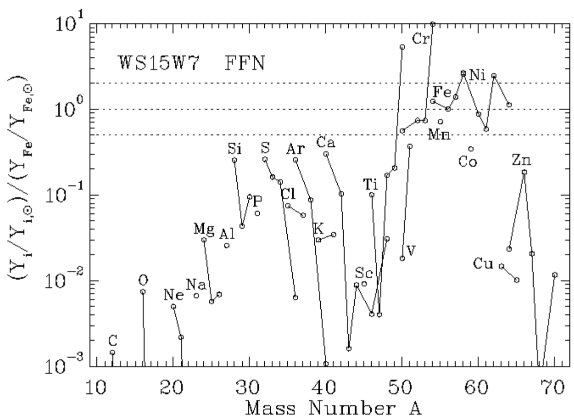
The science:

- ***Chandrasekhar mass model explains SN 1a events as thermonuclear explosions of accreting white dwarfs in binary stellar systems.***
- ***Electron gas in the white dwarf is degenerate and has high Fermi energies***
- ***Thus, electron capture plays a role in the explosion and consequent nucleosynthesis of these systems.***

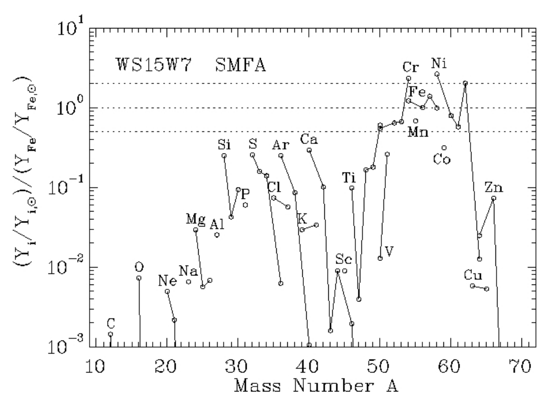
Our Work:

- ***We calculated improved electron-capture rates for iron-group nuclei using Shell Model Monte Carlo techniques and standard shell model diagonalization.***
- ***We demonstrated significant differences in the nucleosynthesis and evolution of the SN using these rates, as shown in the figure.***

Old rates, overproduced Ni and Cr



Our iron region rates, and the vast improvemet in Ni and Cr



Brachwitz, Dean, Hix, Iwamoto, Langanke, Martinez-Pinedo, Nomoto, Strayer, Thielemann, ApJ 536, 934 (2000).

Linear response from TDHF

The science:

- *Various nuclear collective modes may be excited experimentally. Giant-dipole and giant-quadrupole resonances are examples of classical limits of quantum-mechanical motion.*
- *Collective modes may become "soft" as a given isotope becomes neutron rich. The neutron skin may oscillate against the standard nuclear core.*

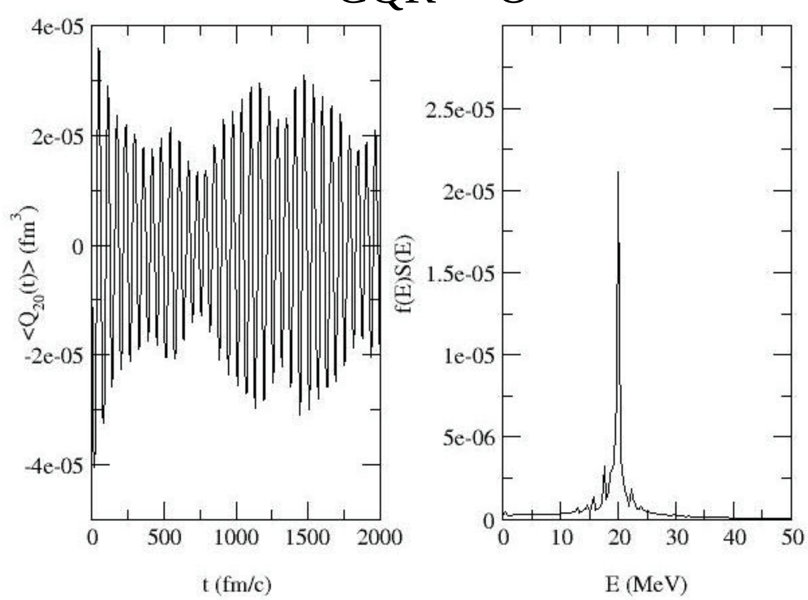
Our Work:

- *We are using TDHF theory to investigate linear response of nuclei to external fields that produce GDR's and GQR's.*
- *We perturb the time evolution with an operator of the form:*

$$Q_{?}^{T}\,?\vec{r},t\,?\,?\;f(t)\,r^{?}\,Y_{?\,0}\,??\;?\hat{n}_{p}\;?\;??1?^{T}\,\hat{n}_{n}\,?$$

- *The Fourier transform yields the strength distribution.*

GQR- ^{16}O



Dean & Strayer

Parallel Shell Model diagonalization Code

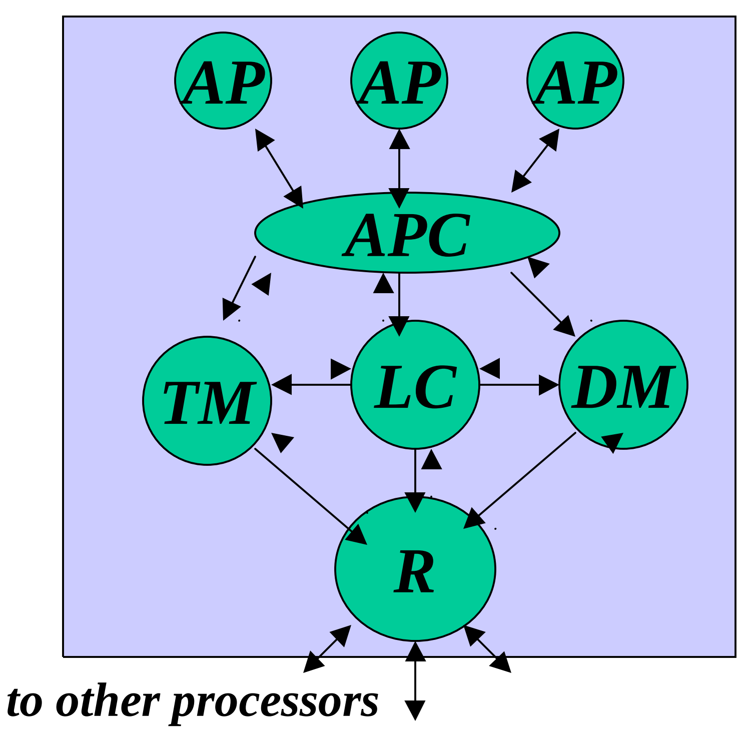
The science:

- Neutron rich nuclei that will be studied at RIA and are now probed at MSU and HRIBF have many active nucleons in the valence space. Understanding the detailed spectroscopy of these systems will require large shell-model diagonalization efforts.
- Experimental efforts to understand the spectroscopy of these nuclei typically requires theoretical guidance.

Our Work:

- To date, no one has developed a scaleable parallel shell model code for distributed memory machines.
  Our goal is to develop a modern shell model code that will perform efficiently on Terascale computational platforms, such as the IBM machines at NERSC and ORNL.

Our computational model for a single processing element.



AP= application process
APC=AP controller
TM=task manager
LC=local controller
DM=data manager
R=router

Juodagalvis, Dean, and Strayer

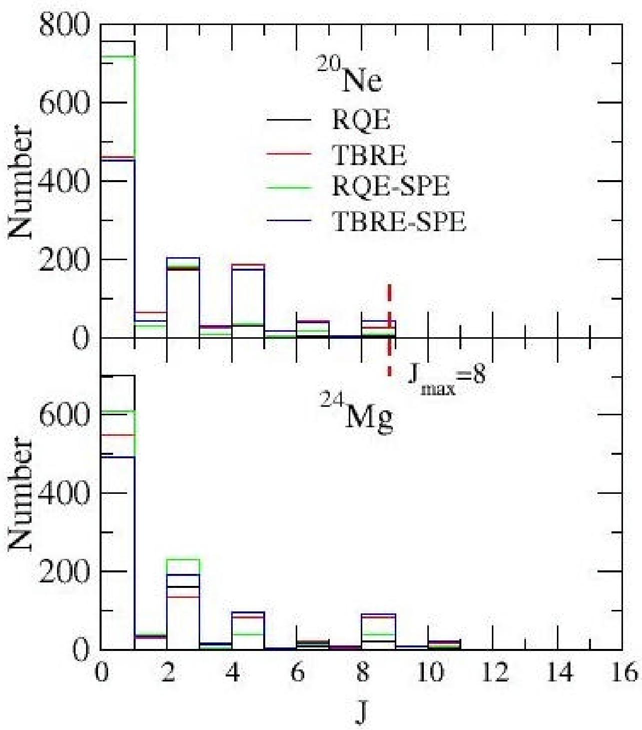
Robust observables from random interactions

The science and our work:

- ***We ask the question: Given a random ensemble of two-body interactions, what characteristics of the nuclear many-body problem remain?***

Robust Feature #1

Enhanced J=0 ground states



Robust Feature # 2

Vibrational and rotational bands exist in the random ensembles (more pronounced in boson-random ensembles).

Robust Feature #3

All random ensembles show enhanced pairing collectivity even when explicit pairing matrix elements (J=0,T=1) are excluded from the ensemble.

Johnson, Bertsch, Dean, PRL80, 2749 (1998)
Johnson, Bertsch, Dean, Talmi, PRC61, 014311 (2000)
Dean, Bennaceur, Ozen, Barmore, Nazarewicz in prep

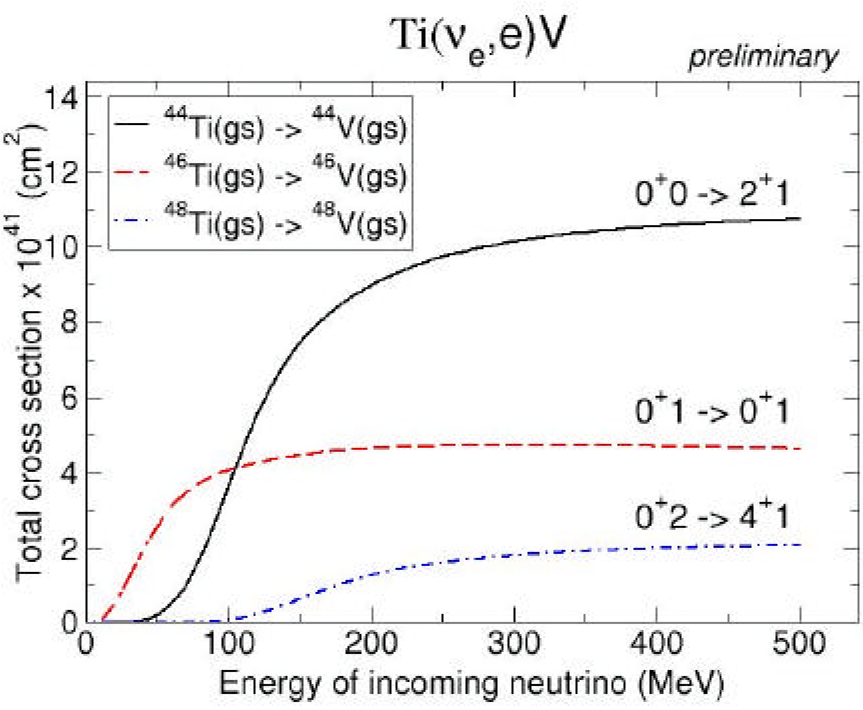
Neutrino-nucleus scattering

The science:

- ***Measurements at ORLaND will give us the opportunity to probe neutrino-nucleus interactions at relatively low energies (<40 MeV).***
- ***Neutrinos play a role supernova evolution, as well as in production of some r-process material.***
- ***In both cases, reliable predictions of cross sections for neutrino-nucleus interactions becomes highly desirable.***

Our Work:

- ***To date, we have developed a code to investigate the weak matrix elements associated with neutrino-nucleus scattering. The input to this code is the density-matrix taken from shell-model calculations.***
- ***Our initial studies are aimed at investigating the cross section dependence as a function of neutrino energy and isotope for a given element.***



Juodagalvis, Dean, Chatterjee, and Strayer

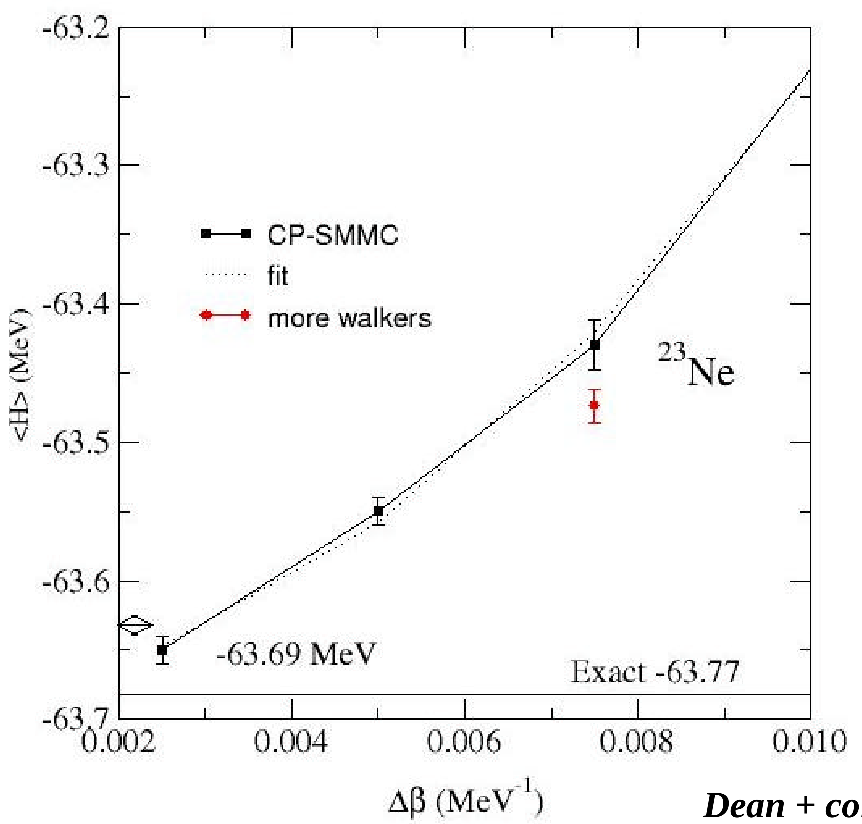
Shell Mode Monte Carlo developments

The science:

- Application of quantum Monte Carlo techniques to the nuclear shell model allows one to explore ground state, rotational, and thermal properties of nuclei by casting the traditional shell-model problem into a path integral.
- Quantum Monte Carlo Methods applied to repulsive interactions engenders a sign problem: the path integrals become highly oscillatory. We often use extrapolation procedures to overcome these problems in nuclear systems.

Our Work:

- In addition to bread and butter calculations, we are investigating methods to overcome the Monte Carlo sign-problem in odd-A nuclei and in the general case of repulsive interactions.



Dean + collaborators

Quantum many-body techniques applied to quantum dots

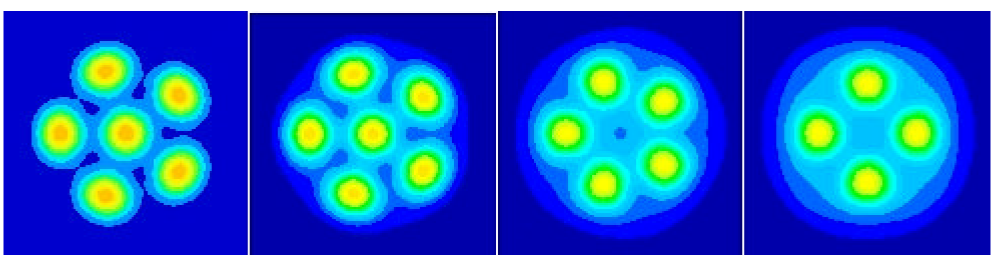
The science:

? ***QD: concept referring to a physical structure which confines electrons in 3D to a size comparable to natural wavelength. “Artificial atoms” can be “tuned” or designed.***

Our Work:

- ***We are studying the properties of few-electron (<20) two-dimensional quantum dots in a varying magnetic field and at finite temperature.***
- ***We are developing Auxiliary Field Monte Carlo (AFMC) techniques to apply to the general problem of electrons confined in two-dimensions.***

Thermal phase transitions at B=16 Tesla.



T=4 K 12 K 13.6K 14.3 K

While the number of electrons remains 6, the number of vortices decreases with increasing temperature. These changes in structure happen rather abruptly as temperature is increased. Thermal properties are experimentally investigated by measuring the chemical potential of the system.

Dean, Strayer, Wells, PRL (submitted, 2000)

LDRD: Computational Nanoscience at the Terascale: Self-Assembled Monolayers and Molecular Electronics

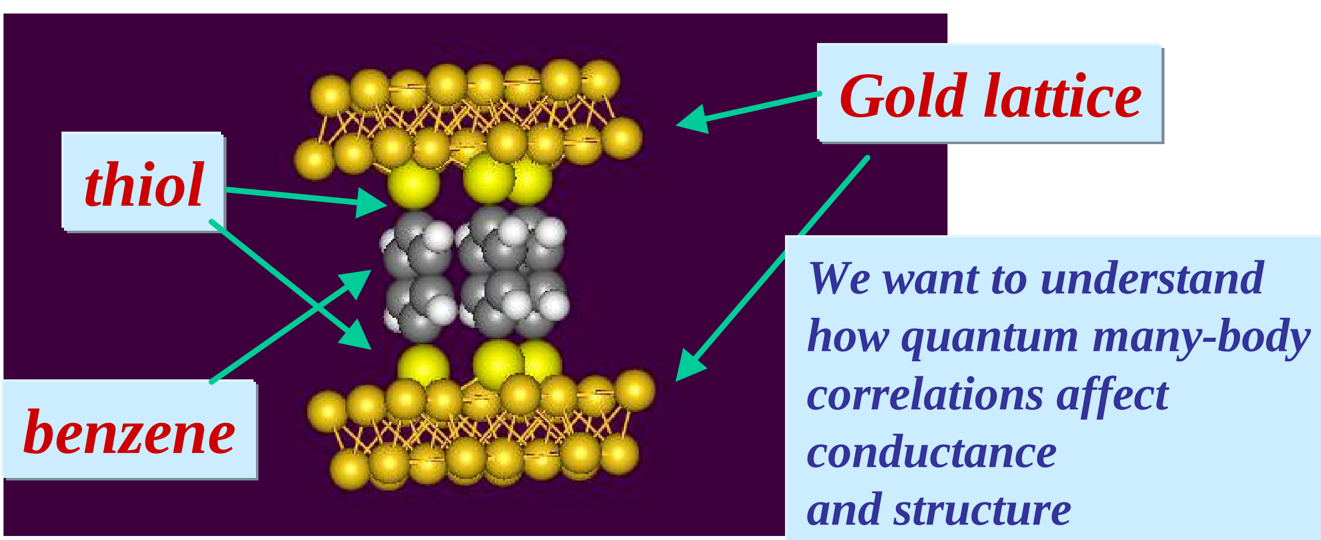
The science:

- Benzene-dithiol molecules attached to gold leads may be used as molecular switches and memory devices in future computational hardware.
- The many-body quantum mechanics necessary to describe electron transport through these devices (induced by an external field) must be well understood if the system is to be controlled.
- Theoretical calculations of conduction are 20-200 times greater than experimental data.

Our Work:

- We are investigating the origin of this discrepancy by
  - a) creating a first principles DFT calculation of the conduction
  - b) utilizing better models for the gold leads
  - c) including many-body correlations in the conduction calculations.

The team: Dean, Strayer, Schultz, Wells, Butler, Cummings, Cui



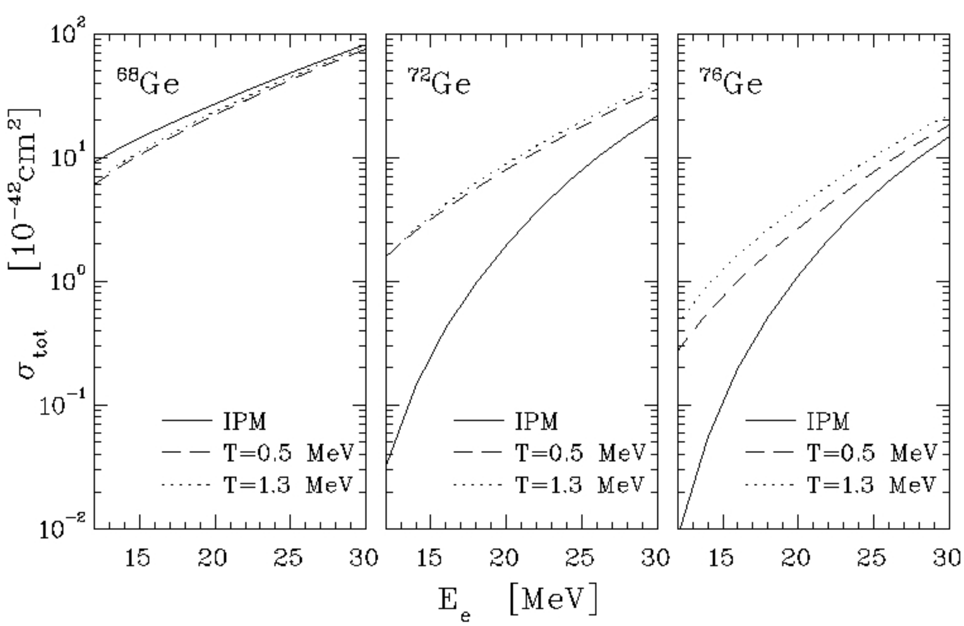
Electron capture on nuclei with N>40.

The science:

- ***Electron capture on neutron-rich nuclei during the core collapse of a massive star.***
- ***In current supernova simulations, electron capture on nuclei is assumed blocked beyond the N=40 shell closure.***

Our Work:

- ***We use SMMC results for occupation probabilities at a given temperature. The Hamiltonian is of the pairing plus quadrupole variety. (Good qualitative effective shell model interactions do not yet exist for this region.)***
- ***We include the occupation numbers as a starting point for RPA calculations of the electron capture rates on N>40, Z<40 nuclei.***



Langanke, Kolbe, Dean, PRC63, 328xxR

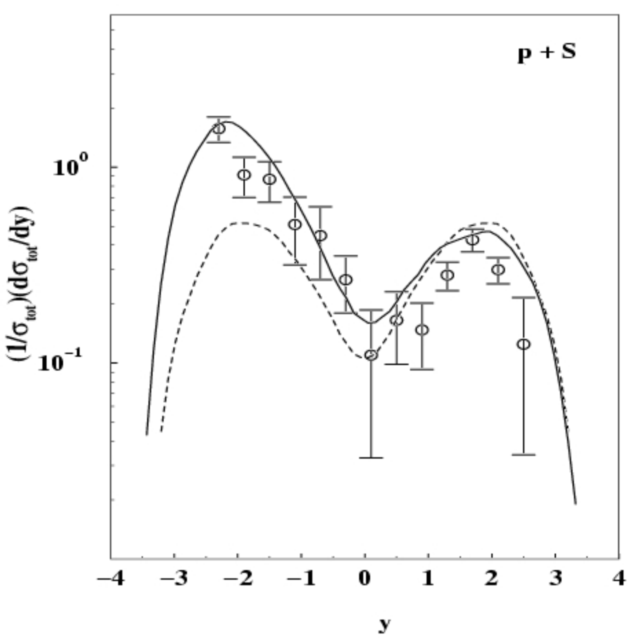
Extensions to the string-parton model of relativistic nucleus-nucleus collisions

The science:

- *Relativistic heavy-ion collisions at sufficiently high energies offers the unique opportunity to probe highly excited dense nuclear matter under controlled laboratory conditions.*
- *Various complicated processes occur during the collision process, including q-q, q-g, and g-g interactions, decay of glue-fields, and freeze-out of produced particles.*

Our Work:

- *We dynamically evolve classical relativistic strings with massless end points. These strings represent the mesons and baryons of our system.*
- *Excited strings decay by virtual pair creation. We enhanced the original model by simulating decay to discrete baryon and meson masses, thus allowing for particle identification in the final states.*
- *Strings interact by end-point scattering. The model incorporates q-q, q-g, and g-g scattering amplitudes.*
- *We applied the model to e-e, p-p, p-A, and A-A collisions.*



Rapidity distribution of net nucleons for minimum bias p+S collisions at 200 GeV/nucleon (solid line, SPM, dotted line p+p, circles, data).

See Malov, Umar, Ernst, and Malov (PRC63, 024902 (2001).

Theory of proton emitters

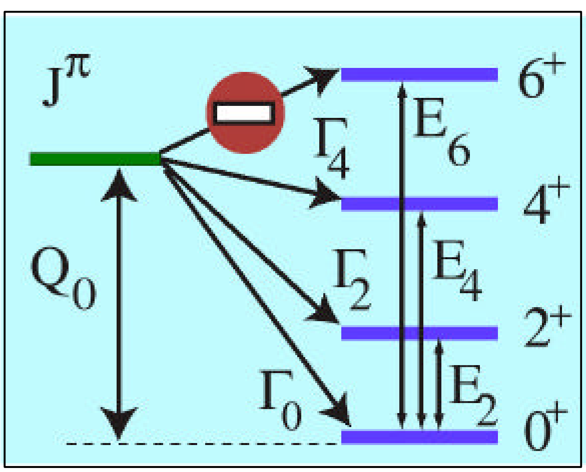
The science:

- *Nuclei beyond the proton dripline are unstable against proton emission. Some of these systems have rather long lifetimes, ranging from ? sec to sec due to the confining effect of the Coulomb barrier.*
- *The past few years have seen an explosion of exciting discoveries in this field (some from HRIBF) including new ground-state and isomeric proton emitters and fine structure in the proton decay.*
- *Theoretically, the main challenge is to understand extremely narrow resonances (quasi-bound states).*

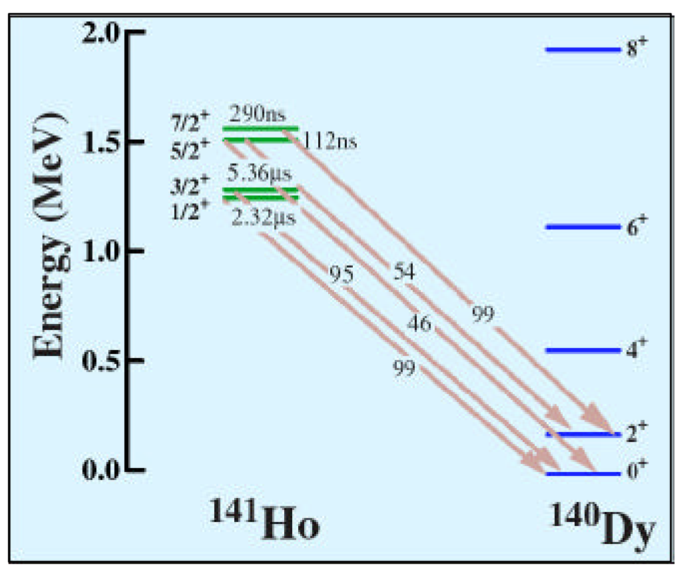
Our Work:

- *We proposed new nonadiabatic theory, based on the coupled-channel equations with Gamow states, to describe narrow resonances in deformed nuclei.*
- *We explained the structure of spherical and deformed proton emitters found experimentally.*
- *We are extending this model to describe electron emission from multiply charged metal cluster anions.*

Energetics of proton emission



Calculated proton emission from ^{141}Ho



A.T. Kruppa, B. Barmore, W. Nazarewicz, and T. Vertse, Phys. Rev. Lett. ***84****, 4549 (2000)*

B.Barmore, A.T. Kruppa, W. Nazarewicz, and T. Vertse, Phys. Rev. C ***62****, 054315 (2000)*

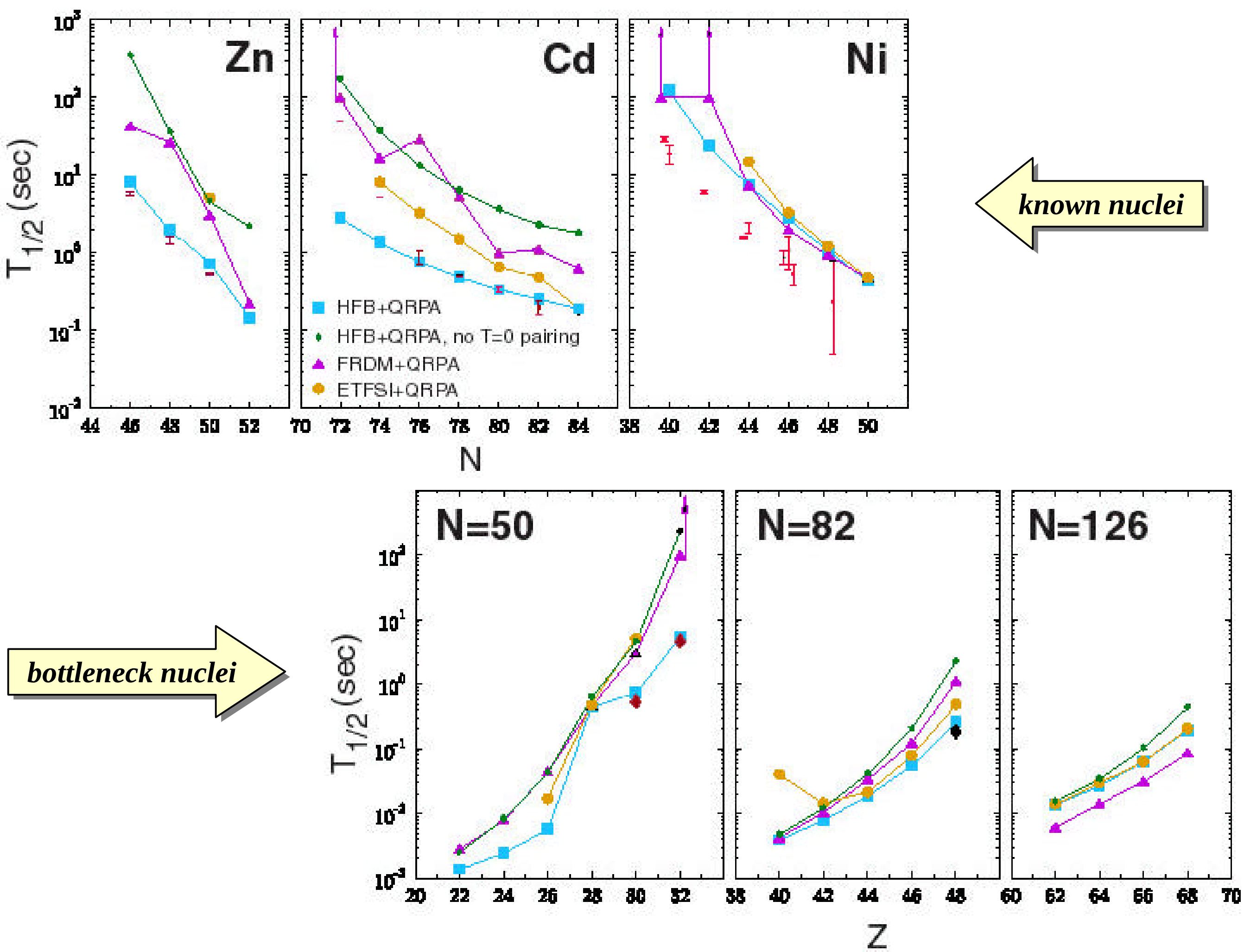
? decay rates of r-process waiting-point nuclei

The science:

- ***The astrophysical r-process, which creates about half of all nuclei with A>70, proceeds through very neutron-rich and unstable isotopes produced by stellar explosions. The ultimate abundance of any stable nuclide depends strongly on ? decay half-lives of its neutron-rich progenitors.***
- ***Understanding the r-process requires knowledge of nuclei far from stability.***

Our Work:

- ***This work contains the first consistent application of the coordinate-space HFB+QRPA formalism to ? ? decay. Our approach fully acconts for the coupling between the nuclear mean field, pairing, and the particle continuum.***
- ***We made detailed predictions lifetimes of semimagic neutron-rich bottleneck nuclei. Our calculations suggest significantly shorter lifetimes than predicted before. This results in an r-process time about 50% shorter.***



J. Engel, M. Bender, J. Dobaczewski, W. Nazarewicz, and M. Surman, Phys. Rev. C ***60****, 014302 (1999)*

Shell effects in superheavy nuclei

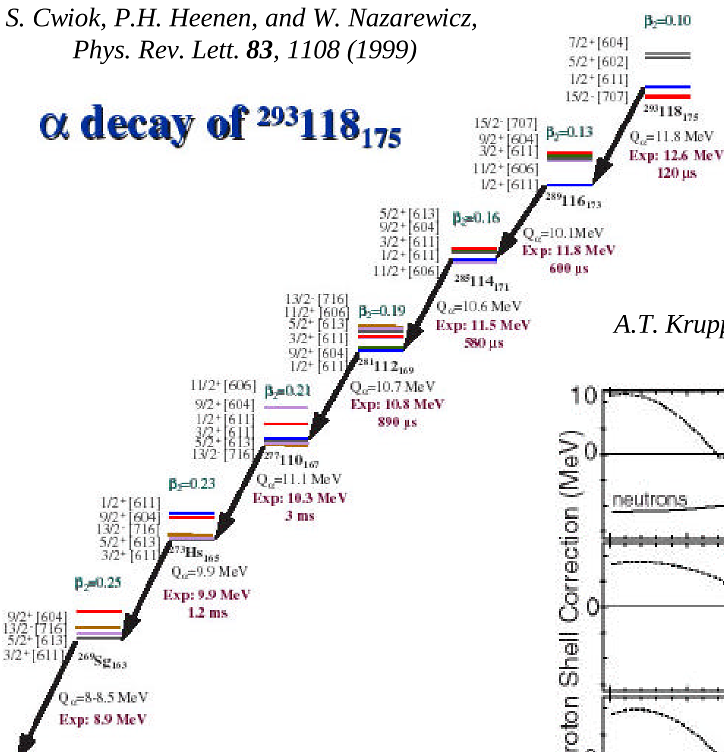
The science:

- *The stability of the heaviest elements has been a long-standing question in nuclear science. Theoretically, the mere existence of the superheavy elements is entirely due to shell effects.*
- *Coulomb energy in the heaviest elements can no longer be treated as a small perturbation.*
- *There are large theoretical uncertainties when extrapolating to unknown nuclei with greater atomic numbers.*
- *There is no consensus among various theories concerning the center of shell-stability above ^{208}Pb.*

Our Work:

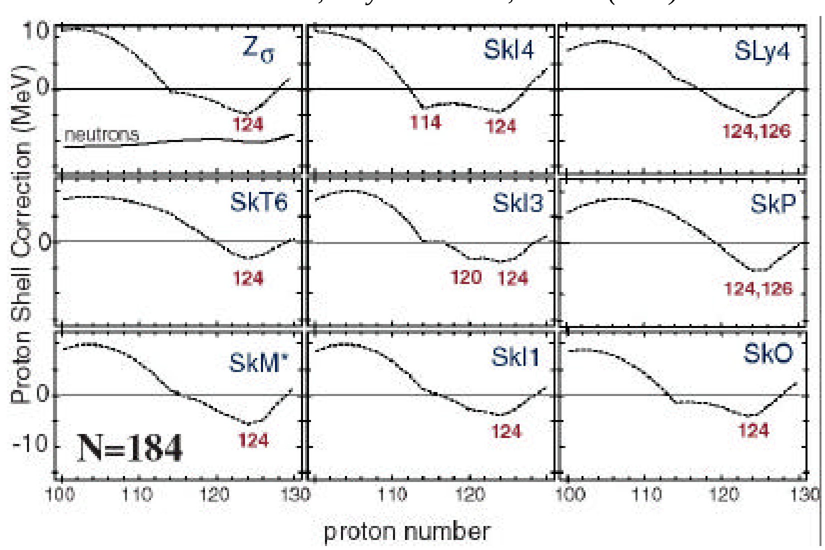
- *We demonstrated that the self-consistent Skyrme calculations predict the strongest spherical shell effect at Z=124,126 and N=184, while the relativistic mean-field theory gives Z=120,N=172. This has important consequences for the question of the spin-orbit force.*
- *We made detailed predictions for the recently observed alpha decay chains of elements Z=118, 114, and 112.*

S. Cwiok, P.H. Heenen, and W. Nazarewicz,
Phys. Rev. Lett. **83***, 1108 (1999)*



Spherical proton shell corrections in the HF-Skyrme model

A.T. Kruppa, M. Bender, W. Nazarewicz, P.G. Reinhard, T. Vertse, and S. Cwiok, Phys. Rev. C **61***, 044326 (2000)*



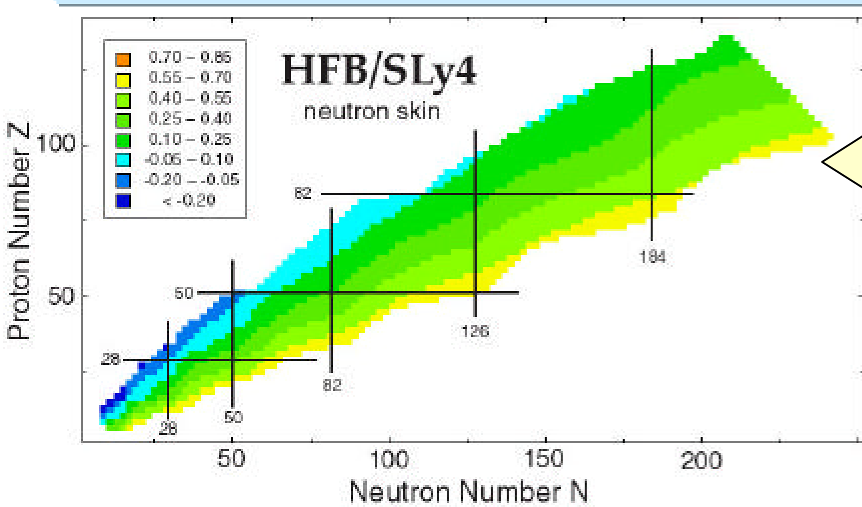
Mean-field description of skins and halos

The science:

- ***Neutron-rich nuclei offer an opportunity to study the wealth of phenomena associated with the closeness of the particle threshold: particle emission, existence of soft modes, changes in shell structure, and surface-dependent superconductivity.***
- ***Neutron-rich nuclei have neutron skins, which manifest themselves in an excess of neutrons at large distances. In addition some weakly-bound nuclei develop very extended halo structures.***

Our Work:

- ***We demonstrated that skins, halos, and surface thickness can be analyzed in a model-independent way in terms of nucleonic density form factors (Helm model). Our analysis allows for a quantitative measure of the halo size.***
- ***We demonstrated that, unlike in the neutron-rich few-body systems, neutron halos do not appear in heavy even-even nuclei. This is because strong pairing correlations significantly influence the asymptotic behavior of the nucleonic density.***

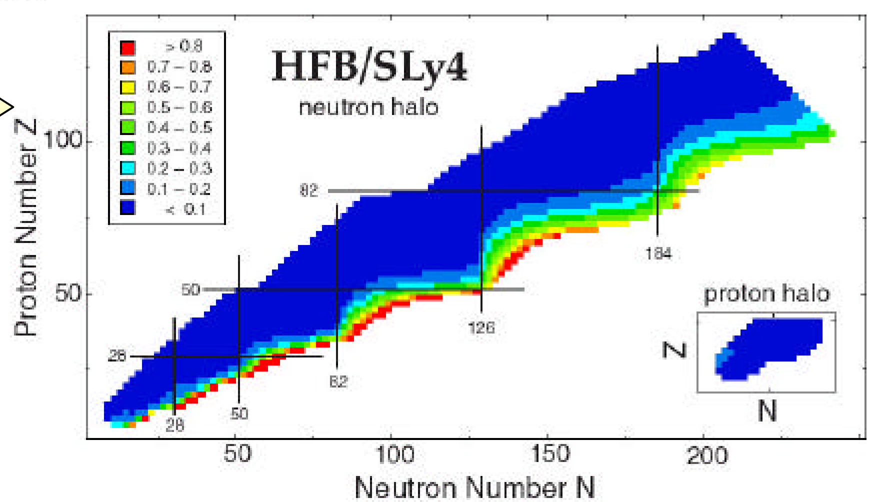


Skin parameters calculated in the spherical HFB/SLy4 model

skin - a bulk effect

Halo parameters calculated in the spherical HFB/SLy4 model

halo - a threshold effect



S. Mizutori, J. Dobaczewski, G.A. Lalazissis, W. Nazarewicz, and P.G. Reinhard, Phys. Rev. C ***61****, 044326 (2000)*

Exact solutions for interacting boson systems under rotation

The science:

- Vortices in atomic Bose-Einstein condensates are presently studied in experiment and theory.
- Analytical expressions for selected wave functions and energies were obtained in the regime of large coherence length.
- Understanding of this solvability missing.

Our Work:

- We explained the solvability in terms of an invariant subspace structure in Hilbert space.
- Results generalize to two-body potentials of zero range and interactions that are analytical in the inter-particle distance squared.

T. Papenbrock and G. F. Bertsch, J. Phys A 34 (2001) 603.

Rotational spectra of weakly interacting Bose-Einstein condensates

The science:

- *Rotational states of atomic Bose-Einstein condensates with long coherence length are of particular theoretical interest.*
- *Low lying excitations well studied.*
- *Structure of highly excited states unknown.*

Our Work:

- *Investigation of entire rotational spectra with numerical and analytical methods.*
- *Low lying excitations are collective states; high energy states are single-particle excitations.*
- *Found excellent analytical approximations for high-lying excitations.*

T. Papenbrock and G. F. Bertsch, to be published in Phys. Rev. A.

Wave function structure in two-body random matrix ensembles

The science:

- ***Recent theoretical studies of nuclear models with random two-body interactions demonstrated that regular features like J=0 ground state dominance or collective excitations exist in spite of the randomness.***
- ***These new findings led to renewed interest in the origin of nuclear structure.***

Our Work:

- ***We investigated the wave function structure in many-body systems with random two-body interactions.***
- ***The inverse participation ratio of low-lying states exhibits significant deviations from random matrix theory and indicates some degree of wave function localization in Fock space.***
- ***We derived a simple analytical formula that describes our numerical results.***
- ***This shows that wave functions of many-body systems with random interactions exhibit regular features at low spectral densities, too.***

L. Kaplan and T. Papenbrock, Phys. Rev. Lett. 84 (2000) 4553.

Spin structuire of many-body systems with two-body random interaction

The science:

- Theoretical studies of nuclear shell models with random two-body interactions revealed regular features like J=0 ground state dominance.
- The unexpected occurance of such regular features in random systems requires an explanation.

Our Work:

- We investigated the spin structure in many-body systems with random two-body interactions. This model is simpler than the shell model but allows for analytical insights.
- We observe a spin-0 ground state dominance and give an analytical explanation in terms of the width and shape of the spin dependent density of states.
- Pairing correlations are observed only in the presence of a sufficiently strong one-body force.

L. Kaplan, T. Papenbrock, and C. W. Johnson, Phys. Rev. C 63 (2001) 014307.