Nuclear Theory in the Supercomputing Era –(NTSE-2016)
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Continuum DFT Studies of Exotic Nuclei and Dynamics

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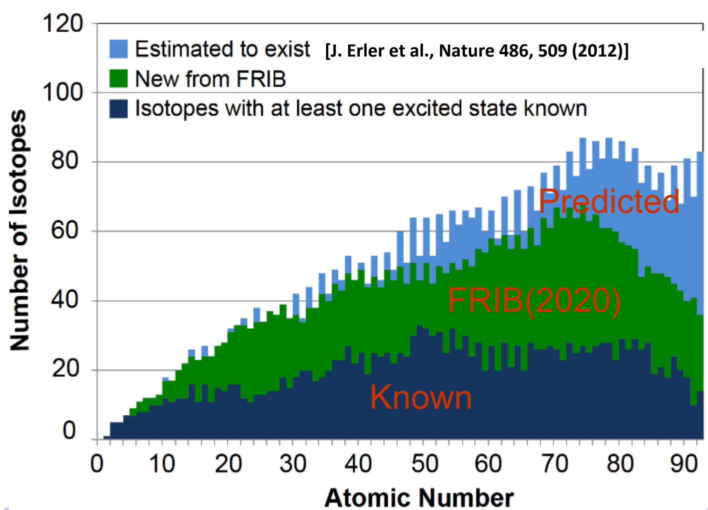
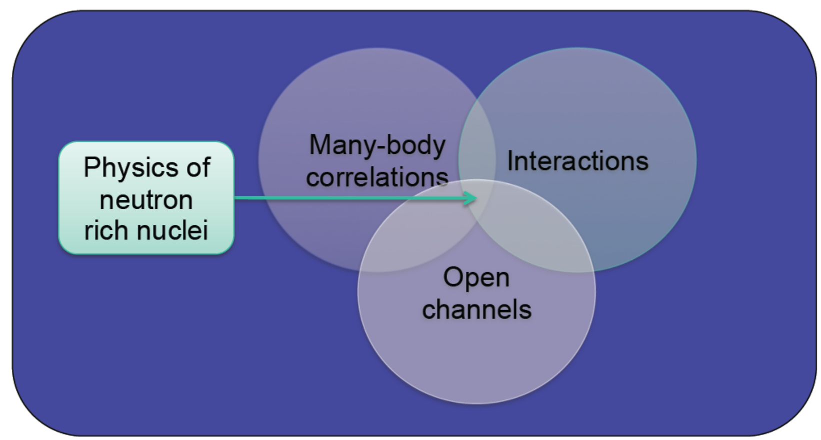
Contents

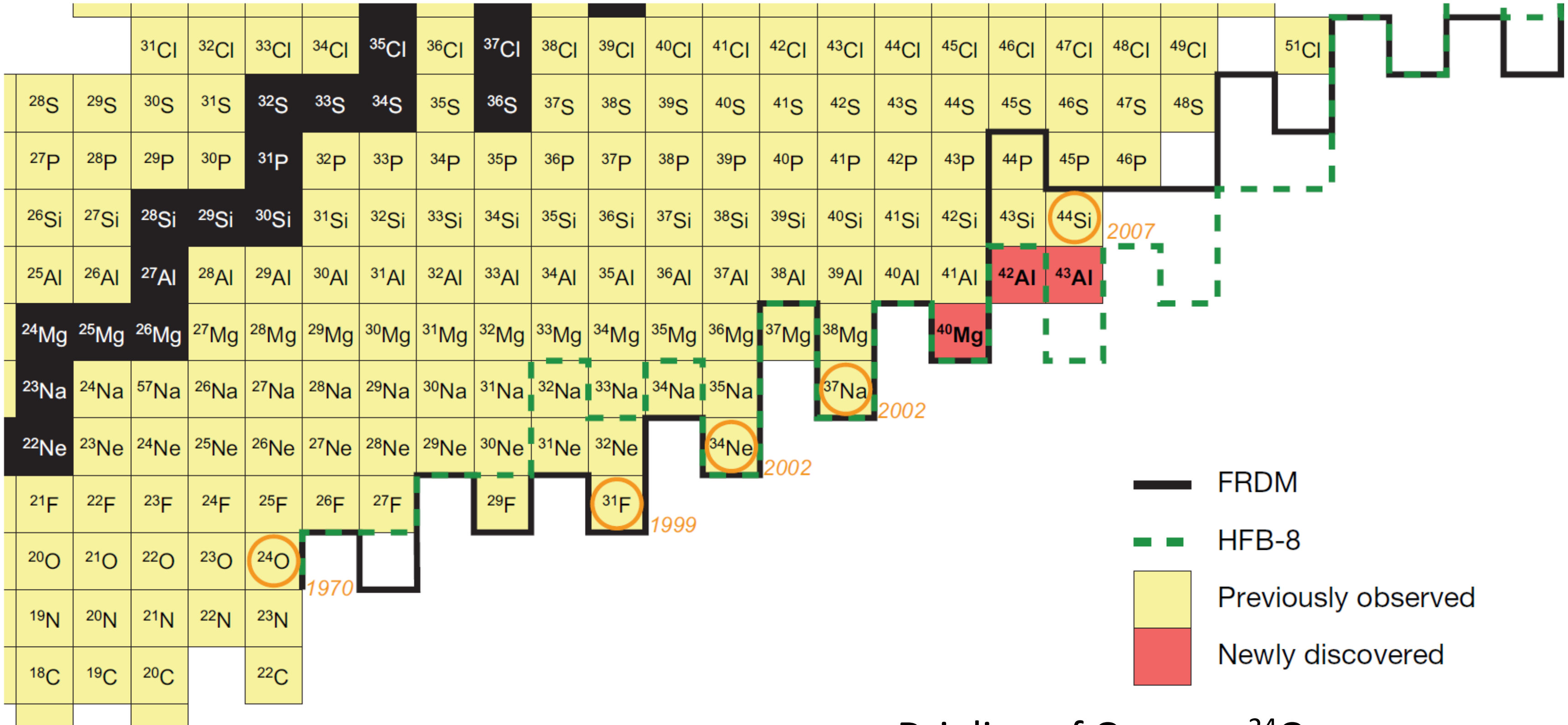
Introduction

- Radioactive nuclear beams (e.g., FRIB, HIAF, Beijing-ISOL) can provide vast opportunities to study nuclear physics at extreme conditions: weakly bound, superheavy, high excitations, high densities
- Interesting physics of dripline nuclei: weakly bound effects, shell evolutions, 3-body forces, continuum effects, soft excitation modes, clustering, breakup, r-process……
- What we can learn from exotic nuclei studies: effective nuclear forces, many-body physics, and new insights.





The dripline



Nature **449**, 1022 – 1024 (25 Oct 2007).

- Dripline of Oxygen: ^{24}O
- RIKEN: (Dec 2014 Expt with 48Ca)

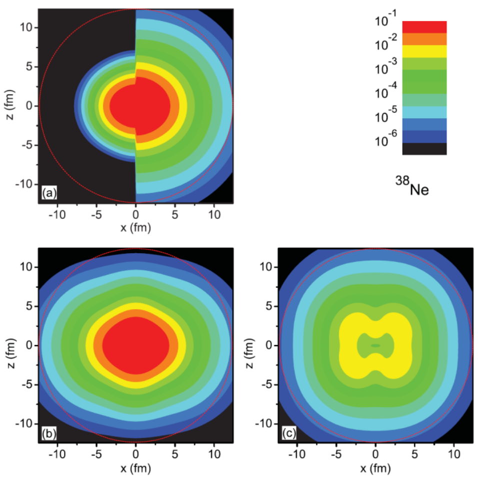
^{33}F(very likely unbound), ^{36}Ne(not found), ^{39}Na(1 event)

Exotic halo structures

- 2D Lattice HFB and MPI+OpenMP parallel calculations

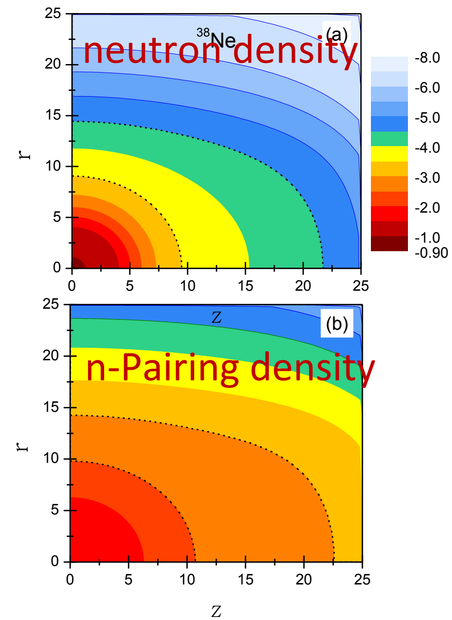
Core-halo deformation decoupling; in principle various halo structures exist

Expt: ^{11}Be,^{31}Ne， and ^{37}Mg

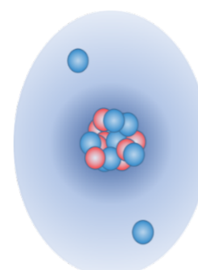


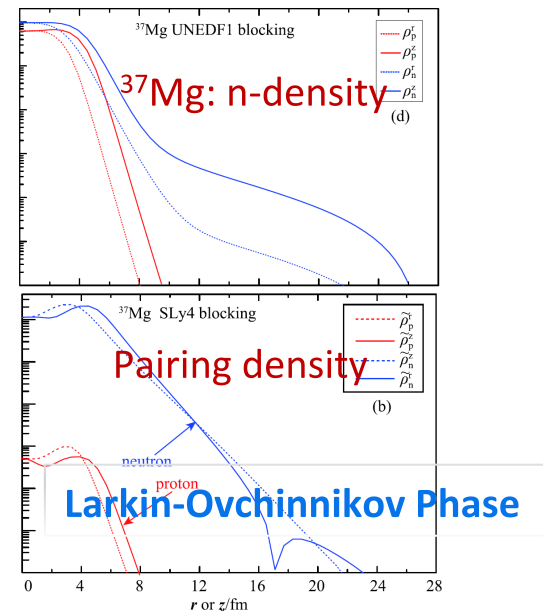
Relativistic Hartree-Bogoliubov
S.G. Zhou, Meng, Ring, Zhao,
2010 PRC 82-011301R

Egg-like halo



Pei ,Y.N.Zhang, F.R.Xu, PRC 87, 051302R(2013)

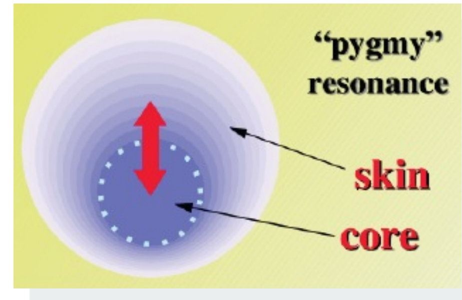


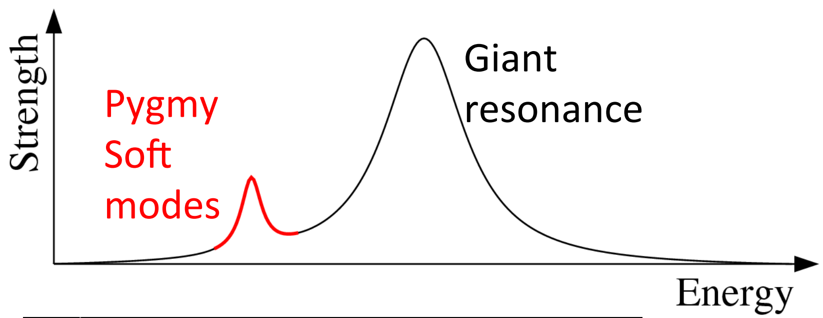


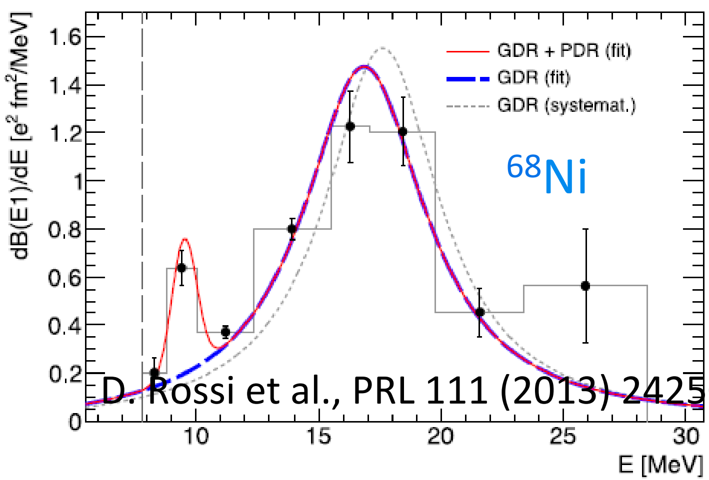
Xiong, Pei, Zhang, Zhu, Chin. Phys. C 40, 024101(2016)

Collective excitations of weakly bound nuclei

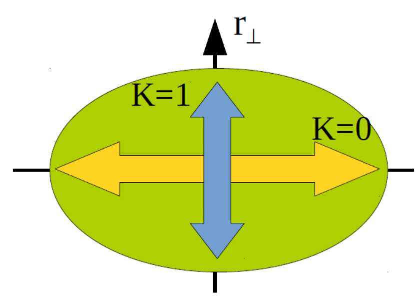
- Novel relative motion between halo/skin and core: collective or non-collective?
- Enhance astrophysical neutron capture rates
- Related to deformation, continuum, neutron skin/halo, symmetry energy, incompressibility…

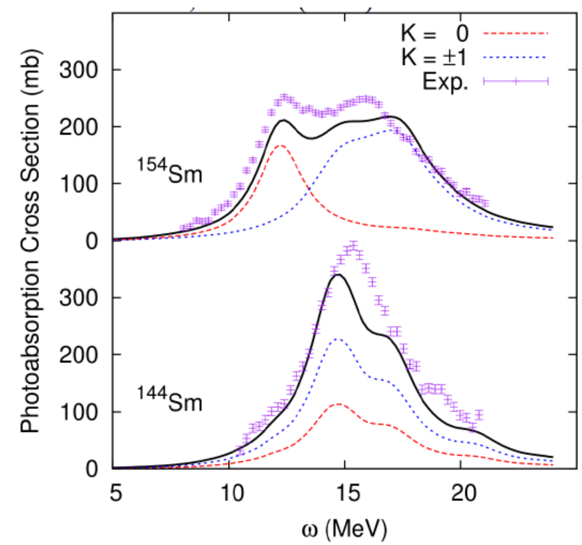






D. Rossi et al., PRL 111 (2013) 242503

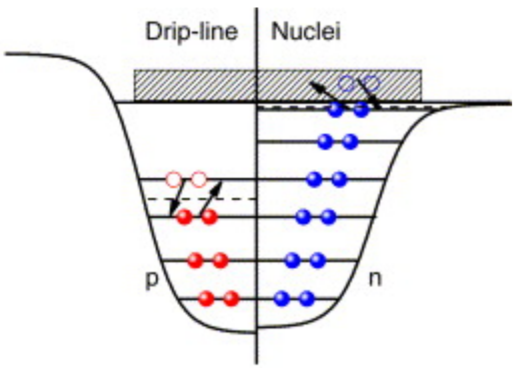


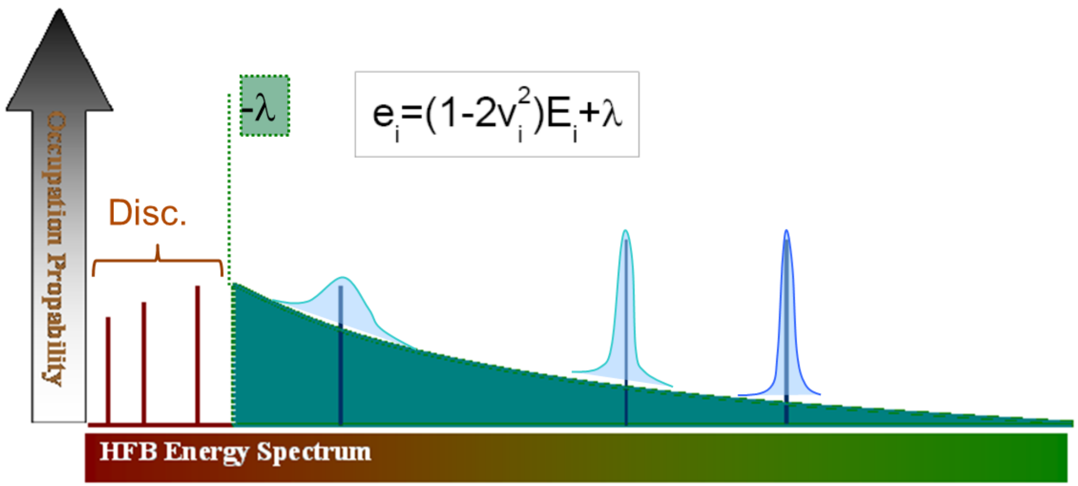


(T. Oishi, et.al, Phys. Rev. C 93, 034329 (2016))

Continuum effects in DFT

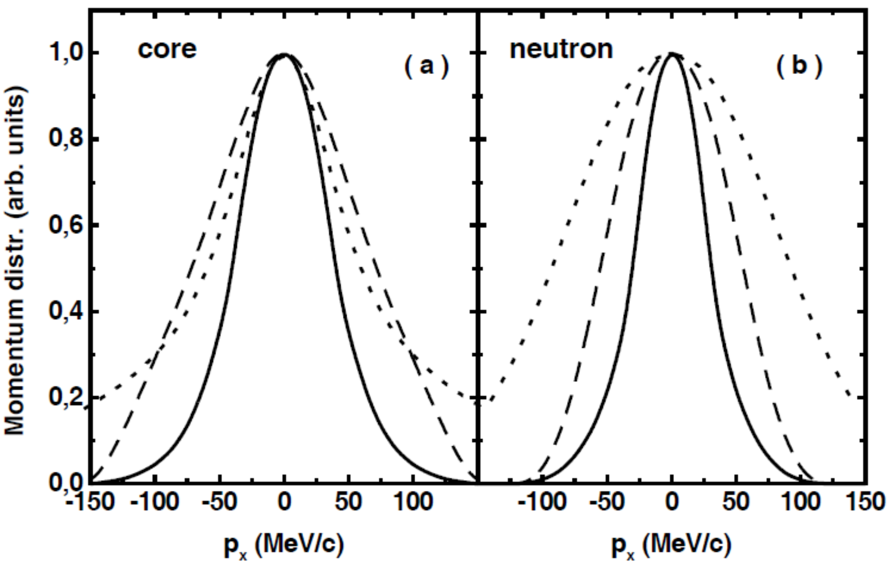
- Continuum coupling: pairing induced
- Weakly-bound s.p. states coupled with continuum: resonances
- Near-threshold non-resonant continuum is important for halos
- Continuum approximation: superfluid Thomas-Fermi approximation
- Enhance stability; enhance halo features; enhance coherent collectivity?

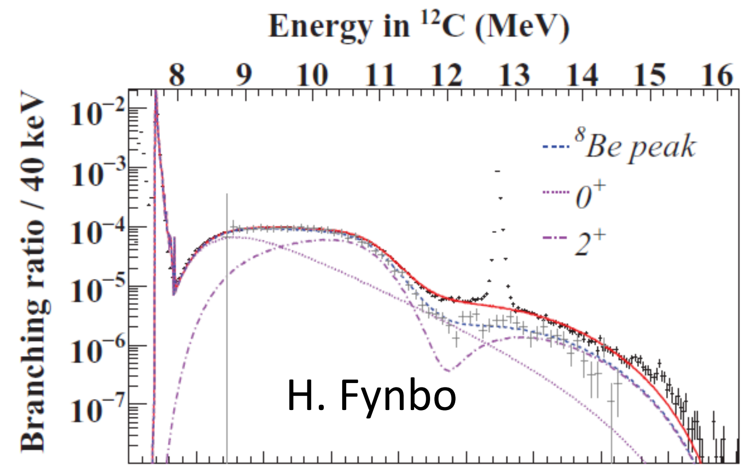


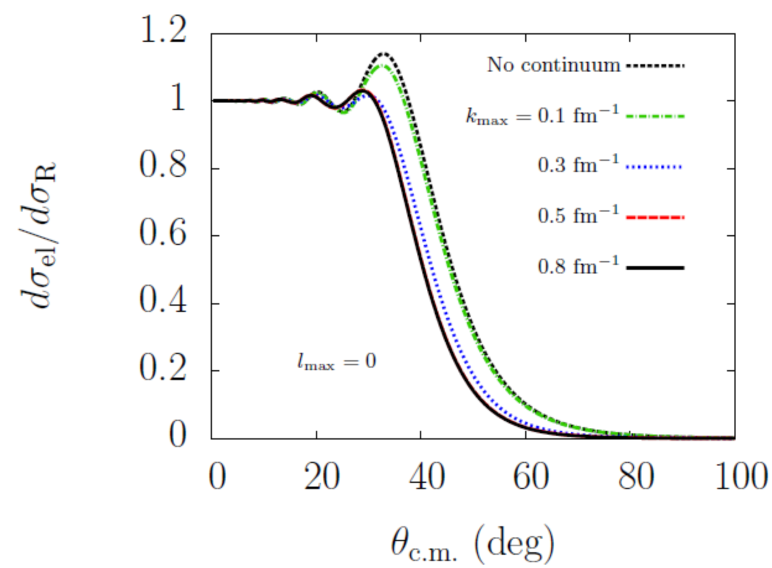


Continuum effects in reaction

- ^{6}He: FSI in momentum distribution
- Breakup, elastic scattering, transfer…
- Continuum effect (ghost) in 12C







S.N. Ershov, et al, PRL 1998
J. Al-Khalili & F. Nunes, JPG 2003
T.Druet, P. Descouvemont, EPJA,2012

Continuum HFB approaches

- Current progress: particularly difficult for deformed weakly bound nuclei

  - Diagonalization on single-particle basis :THO, woods-saxon, PTG, Gamow…
  - Direct diagonalization on 2D coordinate-space lattice (Pei et al, PRC 2008)
  - Outgoing boundary condition: *difficult for deformed cases*

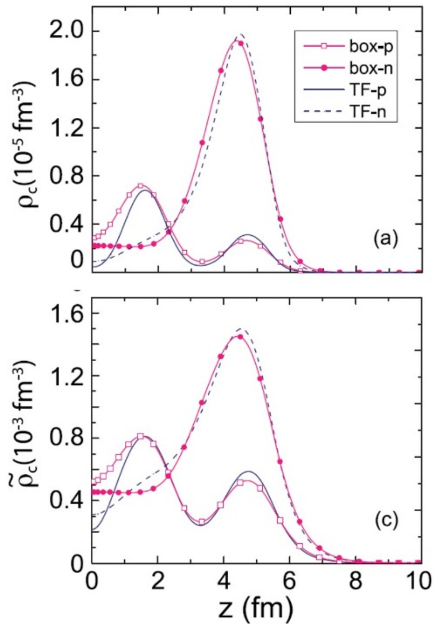
  H. Oba, M. Matsuo, PRC, 2009, self-consistent calculations are needed

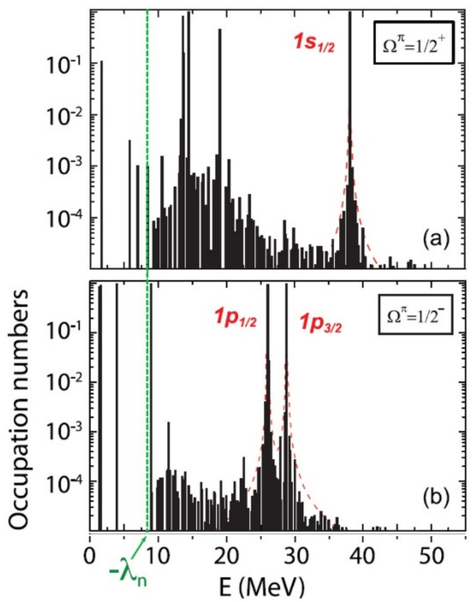
- Coordinate-space HFB has advantages for describing weakly-bound systems and large deformations

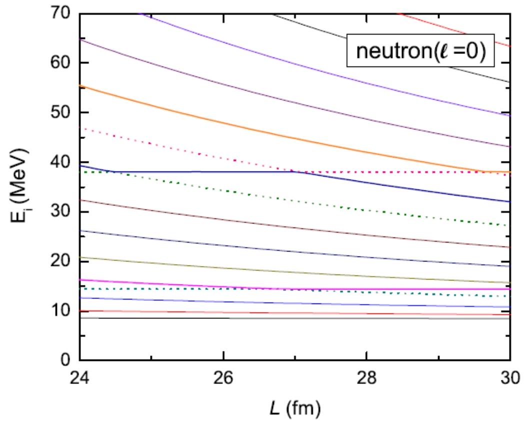
  - *Bound states, continuum and embedded resonances are treated on an equal footing; L^2 discretization leads to a very large configuration space*
  - Computing resources and capabilities are increasing exponentially

continuum discretization treatment

- Non-resonant continuum check with Thomas-Fermi approximation







- Estimate HFB resonance widths with box stabilization method

Pei, Kruppa, Nazarewicz, PRC, 2011

- Problem: broad resonance is expensive

Large vs. small coordinate-spaces

- Subtle interplay among surface deformations, surface diffuseness, and continuum needs precise HFB solutions.
- Large coordinate-space resulted in a vast number of continuum states and provides good resolutions for resonances and continuum (proportional L^3)

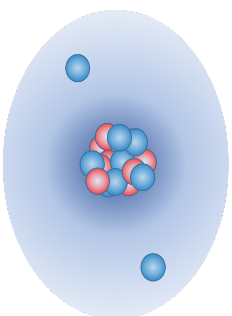
- Small box may not be sufficient for describing halo, pairing properties.
- Small box may be not good for broad resonances.
- Small box may cause false peaks in QRPA

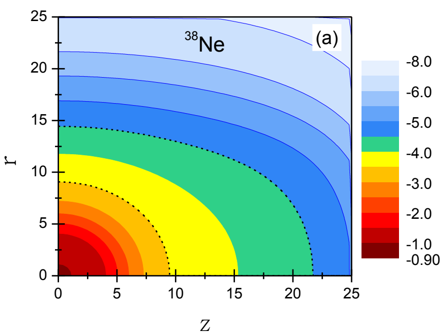
M. Grasso, N. Sandulescu, Nguyen Van Giai, R. Liotta, PRC, 2001.
H. Oba and M. Matsuo, PRC, (2009)
Zhang, Pei, Xu, PRC,2013

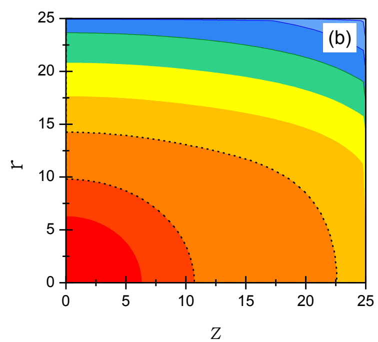
However, from 20 fm to 40 fm, the estimated computing cost would be increased by 40 times.

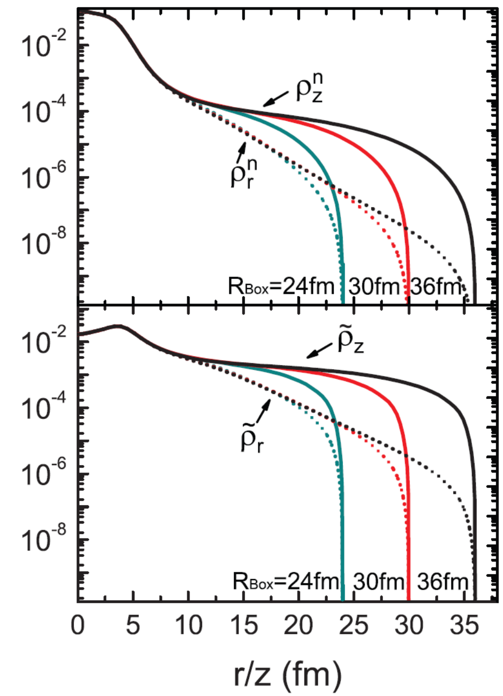
Exotic egg-like halo structure

- Self-consistent calculations: SLy4 force + density dependent pairing
- 38Ne, (a) neutron density; (b) n pairing density
- About 2 neutrons in the halo
- Deformations: beta2 = 0.24, beta2_pair=0.48
- Mainly contributed by near-threshold continuum









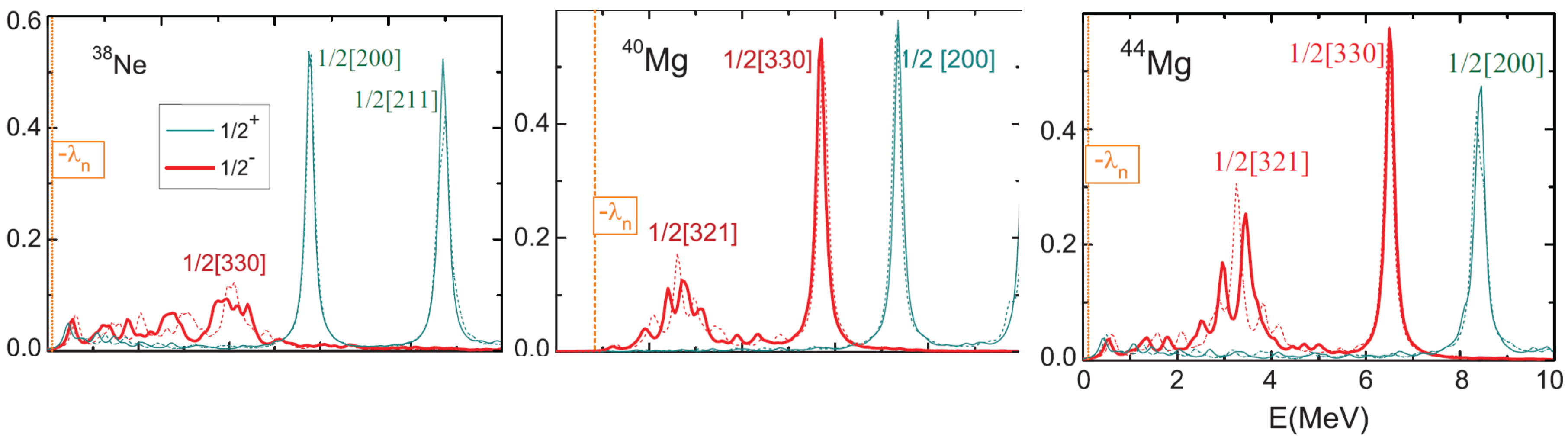
Isovector deformation: pygmy quadrupole resonances

New exotic "egg"-like halo structure obtained; accurate approach is essential

J.P., Y.N. Zhang, F.R. Xu, PRC (R) 87, 051302(2013)

Near-Threshold Continuum

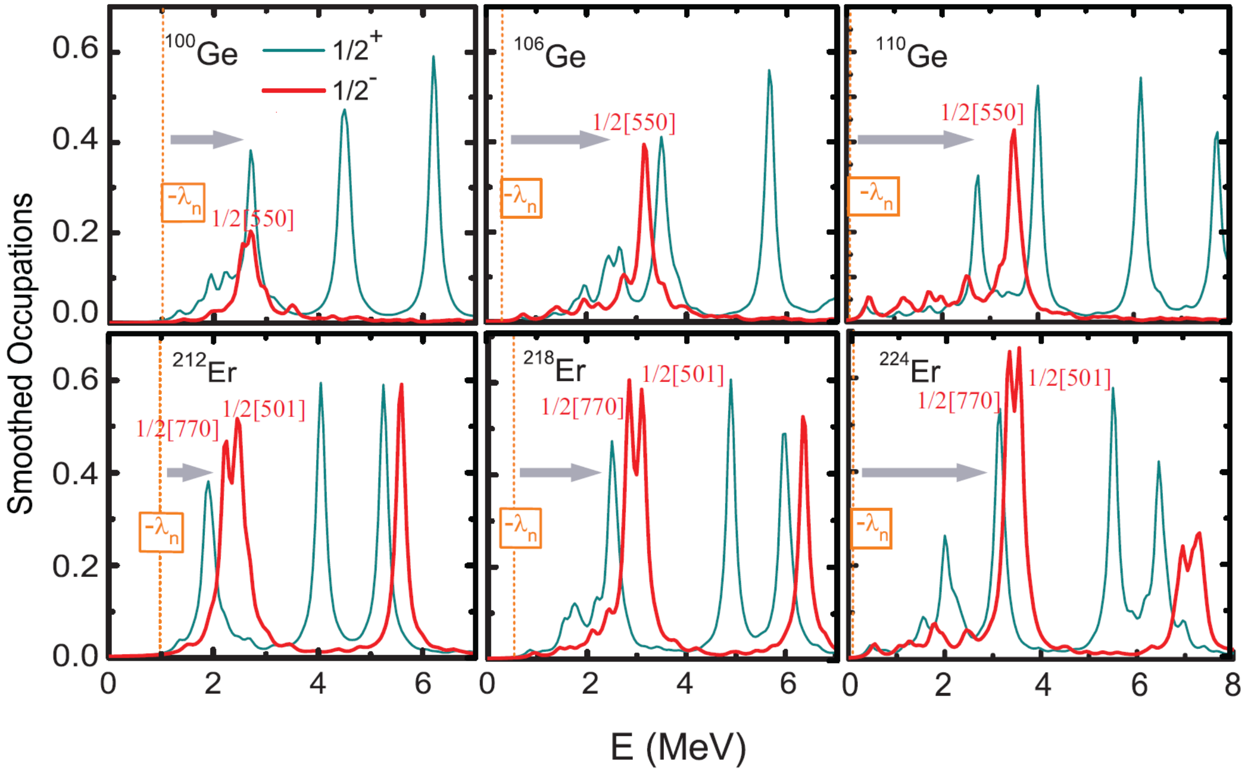
- Different box calculations to distinguish resonances and continuum states
- Near threshold non-resonant continuum is responsible for halo and surface deformations
- No halo in ^{40}Mg since no near-threshold continuum contributions (N=28)



Smoothed neutron quasiparticle spectrum of $\Omega\pi$=1/2$\pm$

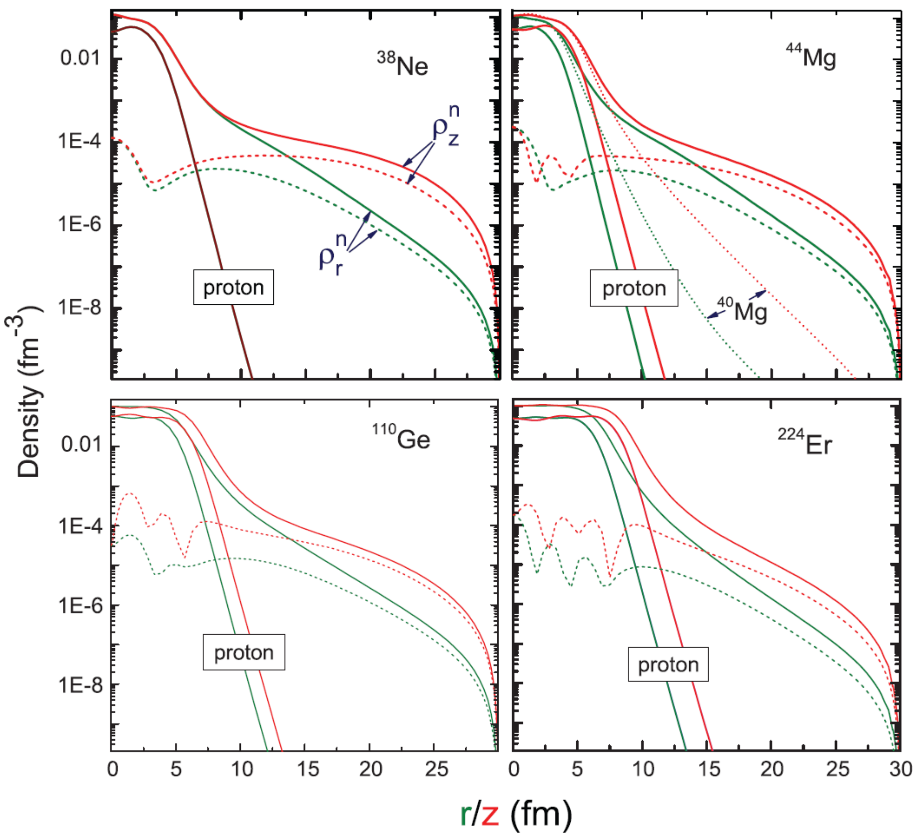
Phase-space decoupling

- Non-resonant continuum states gradually grows and decouples in heavy nuclei
- sparse level density is crucial; e.g. in ^{110}Ge. Heavy halos are hindered due to denser levels.
- Core-halo decoupling is related to the phase space decoupling in quasiptaricle spectrum



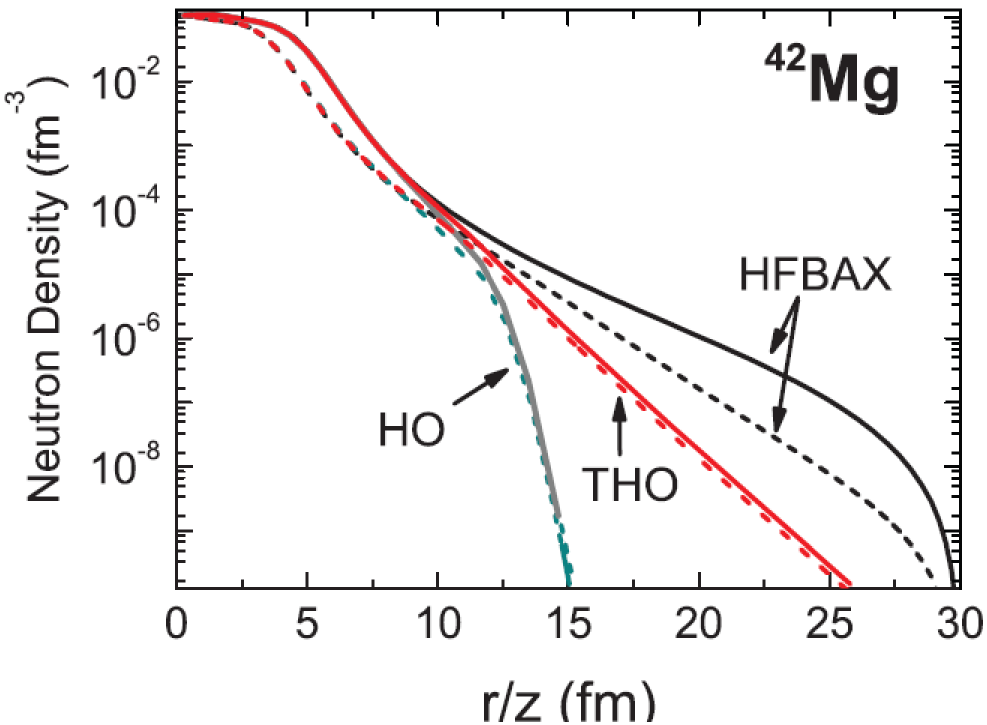
Systematics of deformed halos

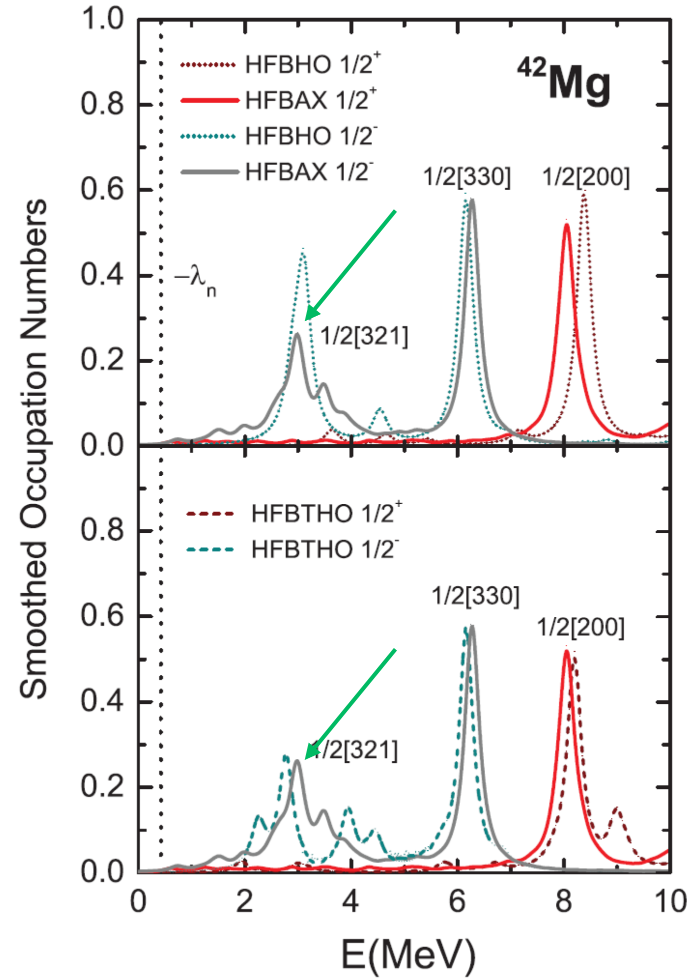
- 2n-Halo hindered by deformed cores (seems correct) *F. Nunes, NPA, 2005(3-body model),* while deformed 1n-halo has been observed in 11Be, 31Ne, 37Mg.
- Heavy halos not likely existed; decoupling effect suppressed



Coordinate-space vs Basis expansion

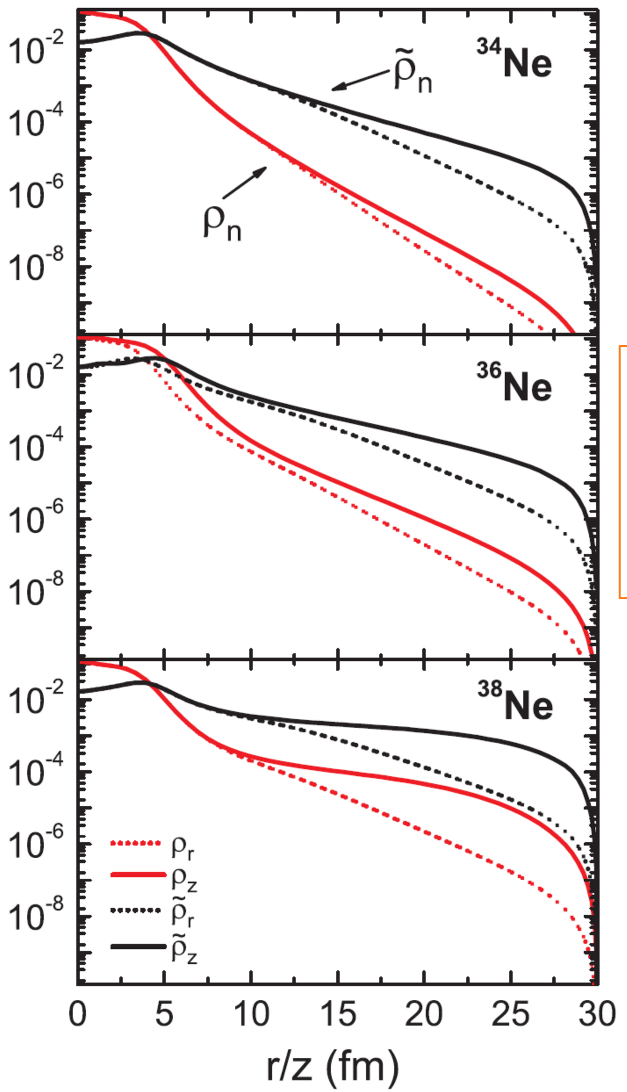
- Different surface asympotics;
- Broad quasiparticle resonance problem



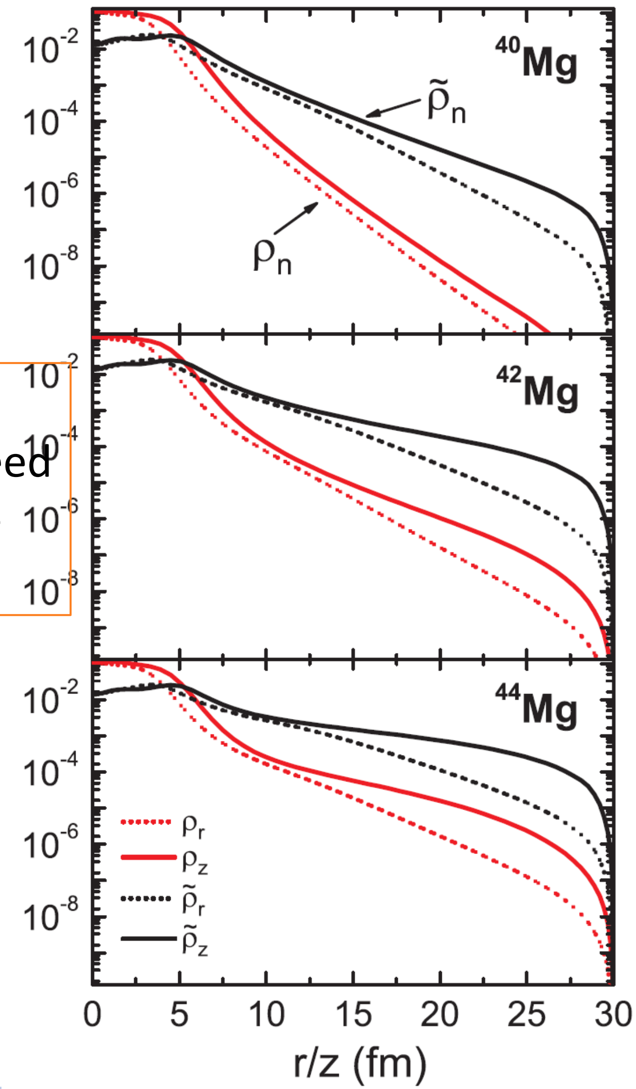


Y.N. Zhang, J.P., F.R. Xu, PRC **88**, 054305, 2013

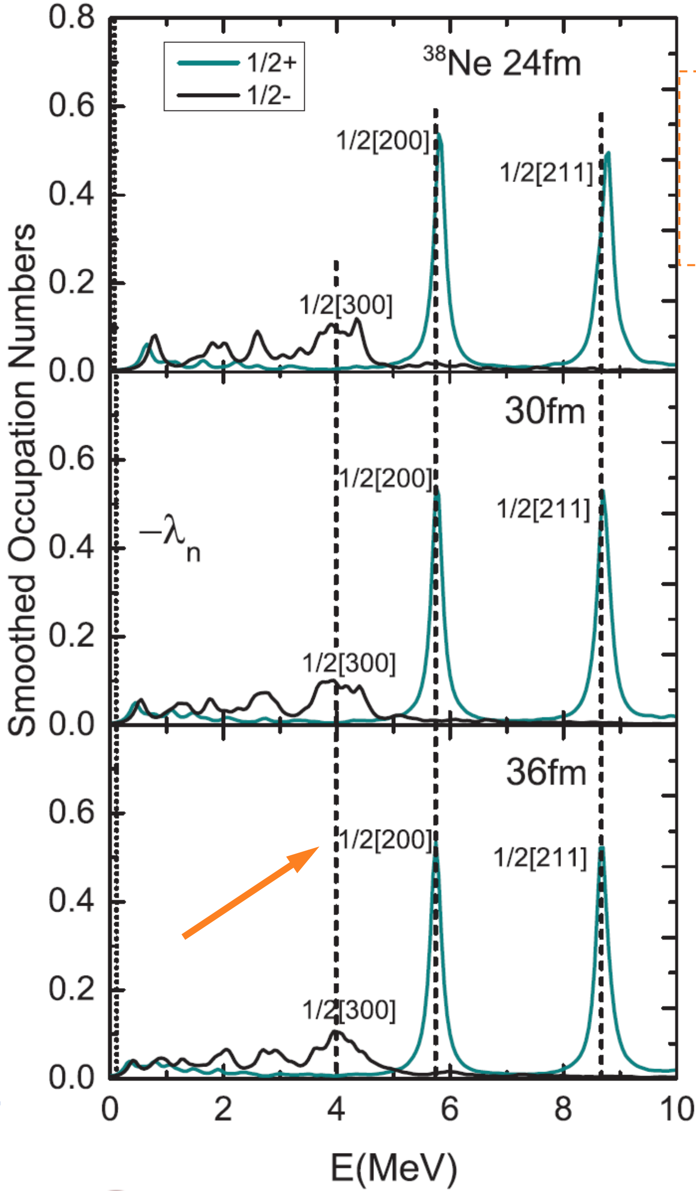
Density and pairing density at surfaces



Huge deformed pairing halos, need large coordinate spaces

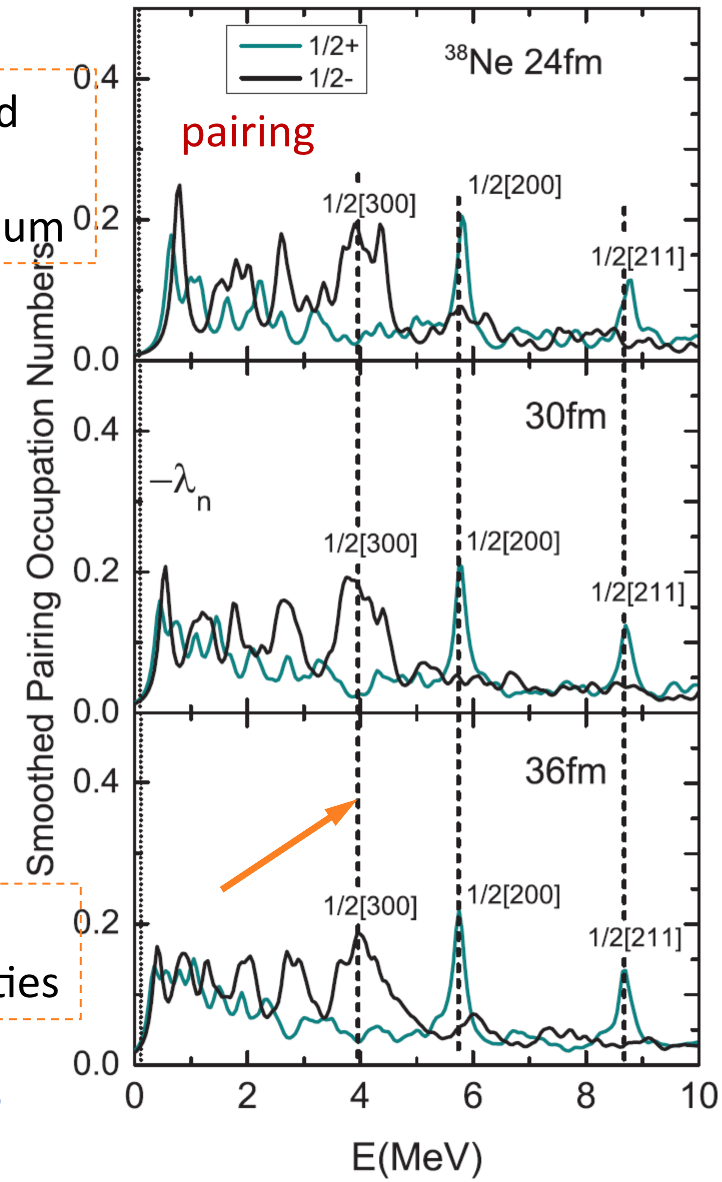


Quasiparticle spectrum near thershold



describing broad resonances and non-res continuum

Problems in pairing properties



2^{nd}-order superfluid Thomas-Fermi

- The 2^{nd}-order Thomas-Fermi becomes complicated with pairing, can be formulated based on Green function expansion
- We derived the 2^{nd} superfluid Thomas-fermi with effective mass and spin-orbit for nuclear calculations of continuum

$$\begin{aligned}
\rho_2(\mathbf{R},\mathbf{p}) = {} & \eta_1(h\overleftrightarrow{\Lambda}^2 h) + \eta_2(h\overleftrightarrow{\Lambda}^2\Delta) + \eta_3(\Delta\overleftrightarrow{\Lambda}^2\Delta) \\
& + \eta_4(h(\overleftrightarrow{\Lambda} h)^2) + \eta_5(h(\overleftrightarrow{\Lambda} h)(\overleftrightarrow{\Lambda}\Delta)) \\
& + \eta_6(h(\overleftrightarrow{\Lambda}\Delta)^2) + \eta_7(\Delta(\overleftrightarrow{\Lambda} h)^2) \\
& + \eta_8(\Delta(\overleftrightarrow{\Lambda} h)(\overleftrightarrow{\Lambda}\Delta)) + \eta_9(\Delta(\overleftrightarrow{\Lambda}\Delta)^2) \\
& + \eta_{10}(h\overleftrightarrow{\Lambda}\Delta)^2 + \frac{3h\Delta^2 h_{so}^2}{4E^5},
\end{aligned}$$

Normal density

$$\begin{aligned}
\tilde{\rho}_2(\mathbf{R},\mathbf{p}) = {} & \theta_1(h\overleftrightarrow{\Lambda}^2 h) + \theta_2(h\overleftrightarrow{\Lambda}^2\Delta) + \theta_3(\Delta\overleftrightarrow{\Lambda}^2\Delta) \\
& + \theta_4(h(\overleftrightarrow{\Lambda} h)^2) + \theta_5(h(\overleftrightarrow{\Lambda} h)(\overleftrightarrow{\Lambda}\Delta)) \\
& + \theta_6(h(\overleftrightarrow{\Lambda}\Delta)^2) + \theta_7(\Delta(\overleftrightarrow{\Lambda} h)^2) \\
& + \theta_8(\Delta(\overleftrightarrow{\Lambda} h)(\overleftrightarrow{\Lambda}\Delta)) + \theta_9(\Delta(\overleftrightarrow{\Lambda}\Delta)^2) \\
& + \theta_{10}(h\overleftrightarrow{\Lambda}\Delta)^2 + \frac{(2h^2-\Delta^2)\Delta h_{so}^2}{4E^5}.
\end{aligned}$$

Pairing density

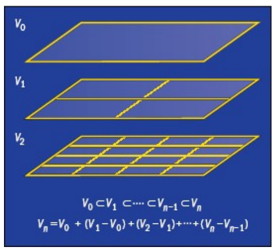
J.C. Pei, Na Fei, Y.N. Zhang, P. Schuck, PRC 2015.

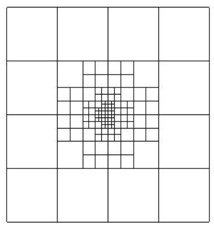
3D Multi-wavelet HFB

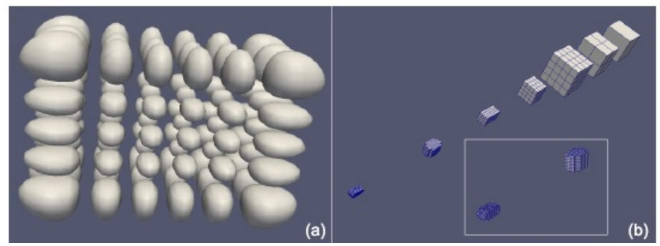
Adaptive multi-resolution 3D Hartree-Fock-Bogoliubov solver for nuclear structure

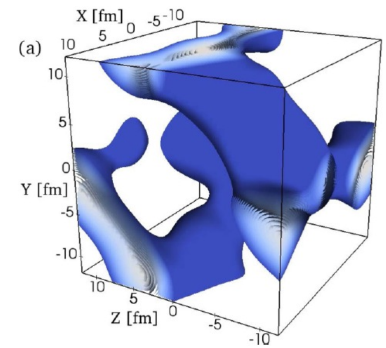
Pei, et al., PRC 2014 (***Editor's Suggestion***)

(Similar to picture compression and computation very efficient)









Nuclear pasta

I. Sagert, et al.,Phys. Rev. C 93, 055801 (2016)

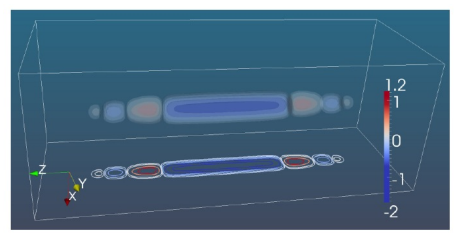
Representations of wave-functions:

$$f^n(x) = \sum_{l=0}^{2^n-1}\sum_{i=0}^{k=1} s_{il}^n \phi_{il}^n(x)$$

Scaling wavelets at V_n
dense and expensive

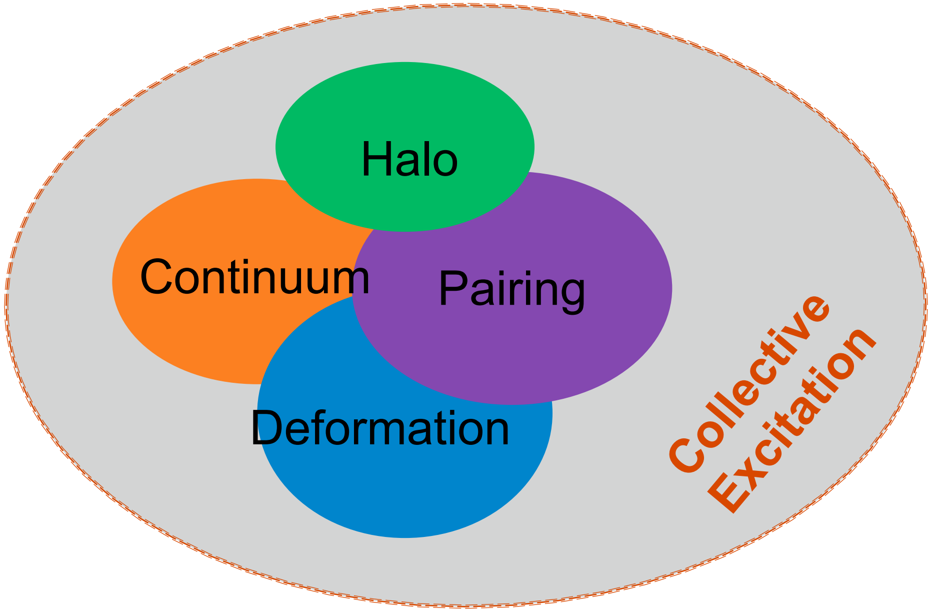
$$f^n(x) = \sum_{i=0}^{k-1} s_{i0}^0 \phi_{i0}^0(x) + \sum_{n=0\ldots}\sum_{l=0}^{2^n-1}\sum_{i=0}^{k=1} d_{il}^n \psi_{il}^n(x)$$

Multi-wavelets
Apply truncation



Trapped Cold Fermi gases

Deformed continuum-QRPA study excited states



- **Great numerical challenge for deformed continuum QRPA**
- Progress in 2013-2014: developed code and benchmark for monopole excitations, including time-odd terms
- Progress in 2015-2016: developed fully code for multiple excitations of deformed weakly bound nuclei

FAM-QRPA

- **Motivation**

Standard QRPA in the matrix form is extremely expensive for deformed nuclei, even more to include continuum configuration

FAM-QRPA provides alternative way solving QRPA equation iteratively rather than diagonalization (FAM-RPA, T. Nakatsukasa, PRC, 2007)

- **Current status of FAM-QRPA**

✓ Based on HFBRAD (spherical coordinate-space HFB), (PRC, T. Nakatsukasa, 2011)

✓ Based on deformed relativistic HB (T. Nikšić, Phys. Rev. C 88, 044327, 2013)

✓ Based on HFBTHO(deformed HO/THO basis) (M. Stoitsov, PRC 84, 2011)

✓ Relativistic FAM-RPA (Liang HZ, PRC, 2013)

✓ Discrete states: N. Hinohara, PRC, 2013

✓ Beta decay: M. T. Mustone, PRC 2014

✓ Multiple FAM-QRPA in HFBTHO, M.Kortelainen, PRC 2015

Implementation in coordinate-space

- HFB-AX output: 2D wavefunctions and energies, quasiparticle basis
  B-spline lattice transformed to Gauss-Legendre lattice
- FAM-QRPA procedure:

1. Construct transition densities (including time-odd terms):

$$\delta\rho(\omega) = UXV^T + V^*Y^TU^\dagger. \qquad \begin{aligned} \delta\kappa^{(+)}(\omega) &= UXU^T + V^*Y^TV^\dagger, \\ \delta\kappa^{(-)}(\omega) &= V^*X^\dagger V^\dagger + UY^*U^T, \end{aligned}$$

$$\left\{ s_\phi,\, j_r,\, j_z,\, (\nabla\times\mathbf{j})_\phi\,,\, (\nabla\times\mathbf{s})_r\,,\, (\nabla\times\mathbf{s})_z\,,\, (\Delta\mathbf{s})_\phi\,,\, T_\phi \right\}$$

$$\begin{aligned} \mathcal{E}_t^{\mathrm{even}} &= C_t^\rho[\rho]\,\rho_t^2 + C_t^\tau\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\nabla J}\rho_t\nabla\mathbf{J} + C^J\mathbf{J}_t^2\,, \\ \mathcal{E}_t^{\mathrm{odd}} &= C_t^s[\rho]\,\mathbf{s}_t^2 + C_t^{\Delta s}\mathbf{s}_t\cdot\Delta\mathbf{s}_t + C_t^T\mathbf{s}_t\cdot\mathbf{T}_t + C_t^j\mathbf{j}_t^2 + C_t^{\nabla j}\mathbf{s}_t\cdot\nabla\times\mathbf{j}_t \\ &\quad + C_t^{\nabla s}(\nabla\mathbf{s}_t)\,, \end{aligned}$$

Implementation in coordinate-space

- 2. Calculate H^{20}, H^{02}(including time-odd terms), F20, etc

$$\delta H^{20}_{\mu\nu}(\omega) = U^\dagger \delta h V^* - V^\dagger \delta\Delta^{(-)*} V^* + U^\dagger \delta\Delta^{(+)} U^* - V^\dagger \delta h^T U^*,$$

$$\delta H^{02}_{\mu\nu}(\omega) = -V^T \delta h U + U^T \delta\Delta^{(-)*} U - V^T \delta\Delta^{(+)} V + U^T \delta h^T V.$$

$$\delta h(\omega) = \frac{h[\rho_\eta, \kappa_\eta^{(+)}, \kappa_\eta^{(-)*}] - h[\rho, \kappa, \kappa^*]}{\eta},$$

$$\delta\Delta^{(+)}(\omega) = \frac{\Delta[\rho_\eta, \kappa_\eta^{(+)}, \kappa_\eta^{(-)*}] - \Delta[\rho, \kappa, \kappa^*]}{\eta},$$

$$\delta\Delta^{(-)}(\omega) = \frac{\Delta[\rho_\eta^\dagger, \kappa_\eta^{(-)}, \kappa_\eta^{(+)*}] - \Delta[\rho, \kappa, \kappa^*]}{\eta},$$

- 3. Calculate X, Y; and Broyden iteration on X, Y. (30 iterations kept)
- 4. Finally calculate the strength

$$X_{\mu\nu} = -\frac{\delta H^{20}_{\mu\nu}(\omega) - F^{20}_{\mu\nu}}{E_\mu + E_\nu - \omega}, \quad Y_{\mu\nu} = -\frac{\delta H^{02}_{\mu\nu}(\omega) - F^{02}_{\mu\nu}}{E_\mu + E_\nu + \omega}.$$

$$S(F,\omega) = \frac{1}{2}\sum_{\mu\nu}\{F^{20*}_{\mu\nu} X_{\mu\nu}(\omega) + F^{02*}_{\mu\nu} Y_{\mu\nu}(\omega)\},$$

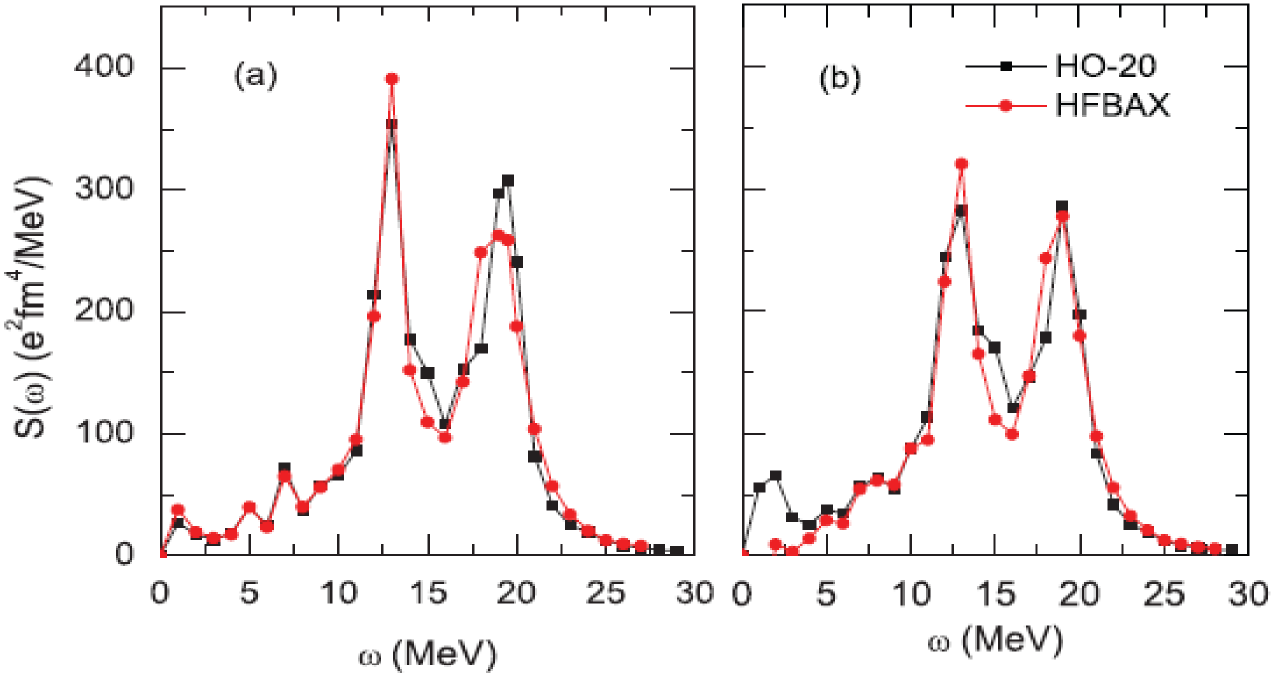
Implementation in coordinate-space

- Combined parallel calculations in TH-1A,TH-22 supercomputers
  for different excitation frequency : MPI distributed parallel
  for each point in a node: OpenMP multi-thread parallel (12 threads)
- Time-consuming: read wavefunctions (10-20 G) and calculate transiton densities and H^{20}, which was a great challenge for matrix-form QRPA.

- Isoscalar monopole modes for soft incompressibility
- Isovector dipole mode for pygmy resonances
- Isoscalar quadrupole mode for proton and neutron differences

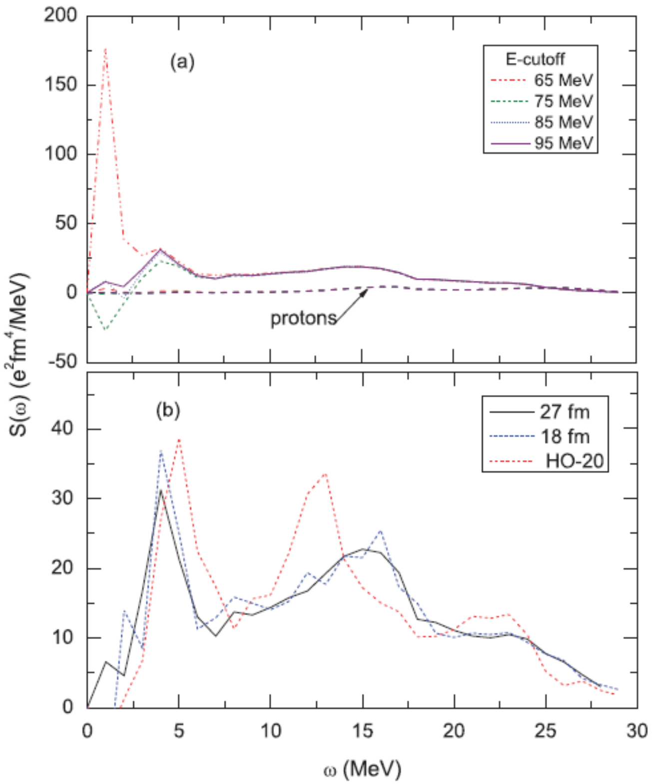
Benchmark with HO basis

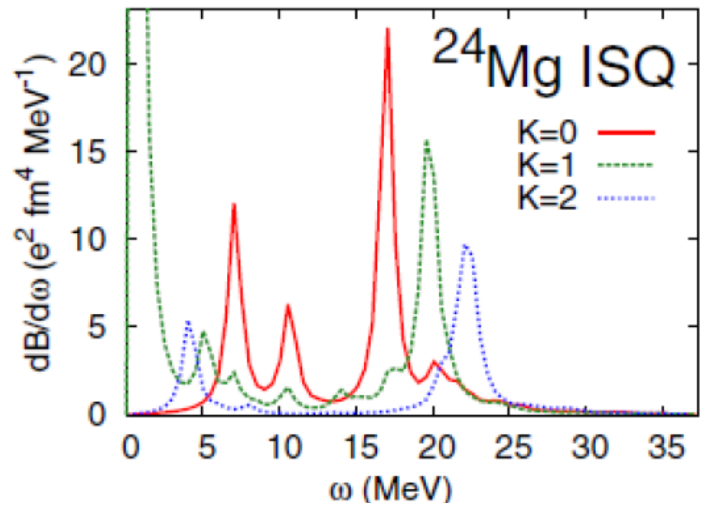
- SLy4+volume pairing and surface pairing (100Zr)

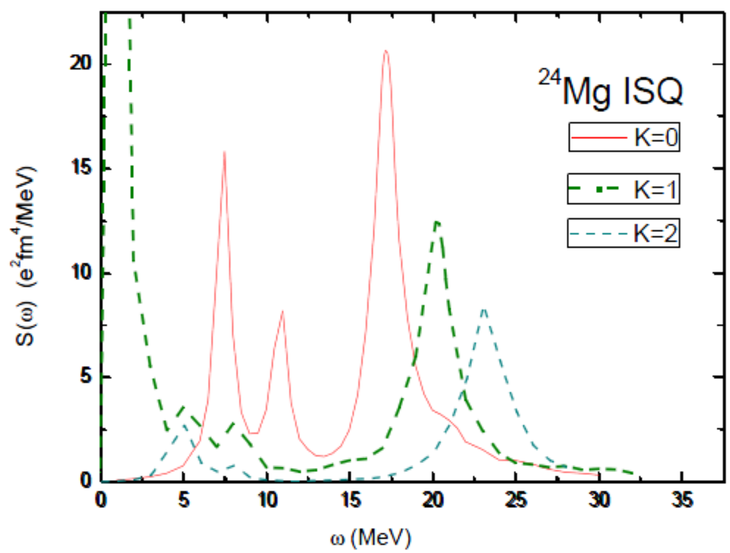


Benchmark with HO basis

- Tests on Cutoff and box sizes
- Spurious modes <= 2 MeV
- Large box is essential



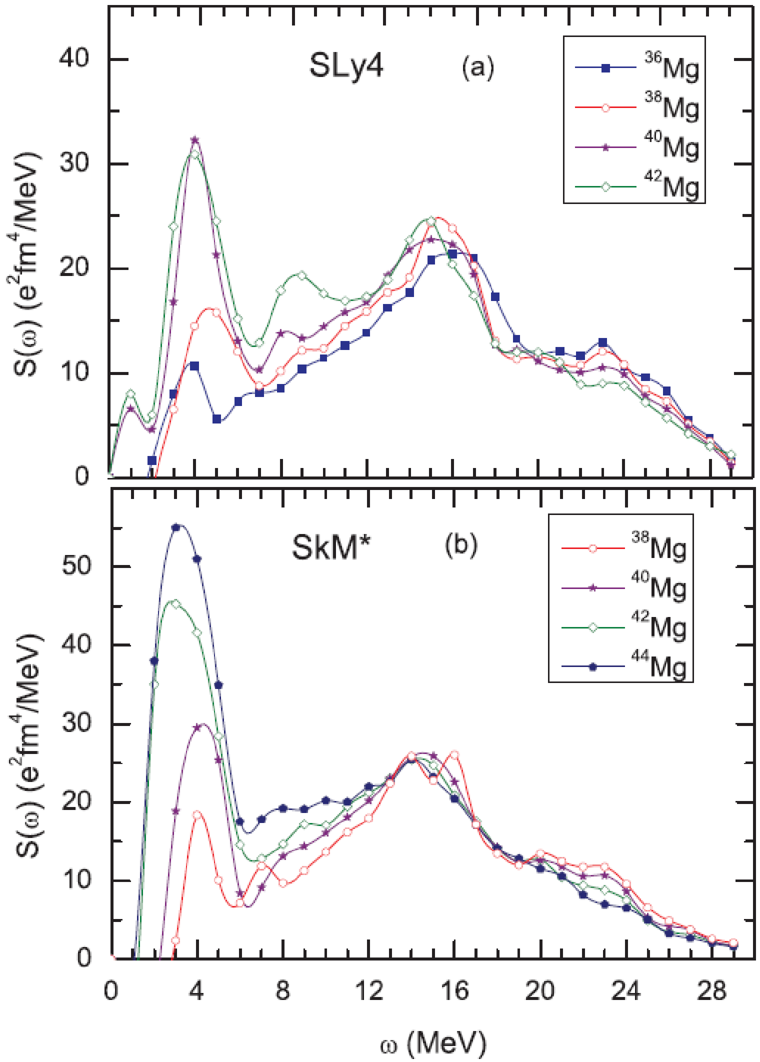




Mg isotopes and soft monopole modes

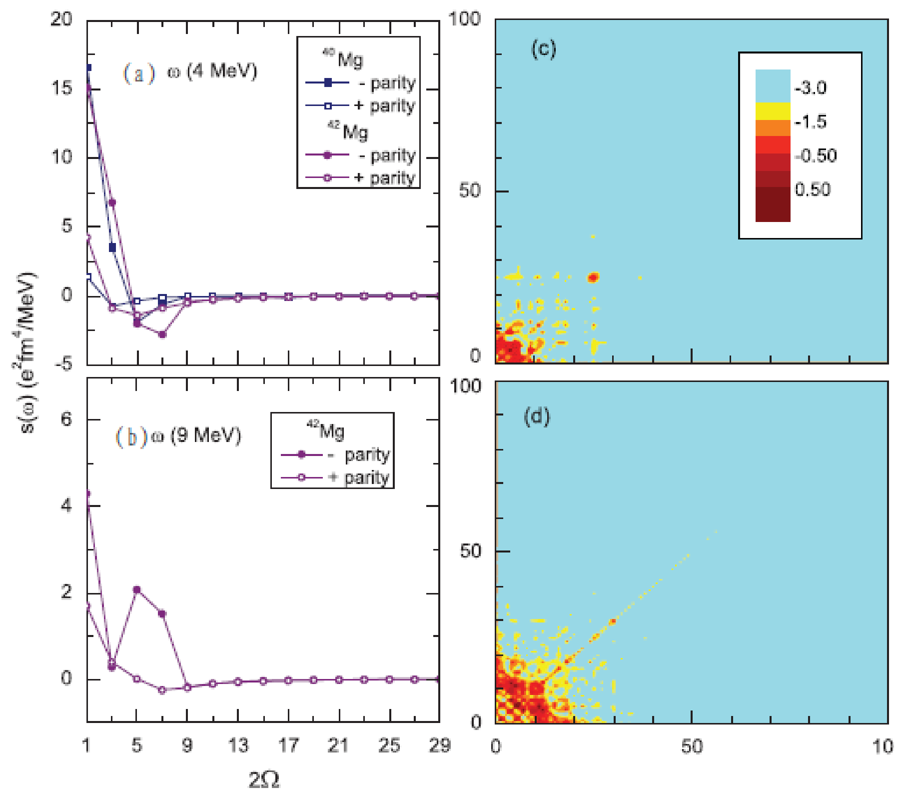
- Soft mode 4 MeV
  close to threshold
  enhanced due to surface pair

- Novel mode 9 MeV
  novel according to systematics
  weak in SkM* calculations



Collectivity and mechanism

- 4 MeV res. collectivity increase
- $1/2^{-}$ states most important
  (also for halo)
- Non-resonant continuum
  (around 2 MeV)
  pairing halo vibrations

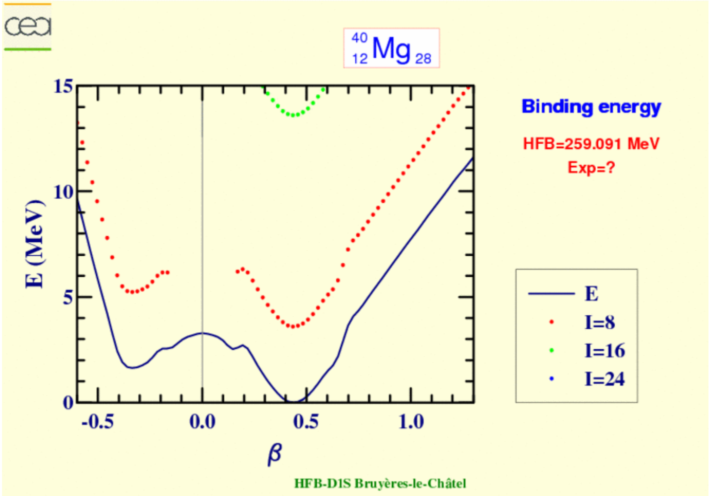


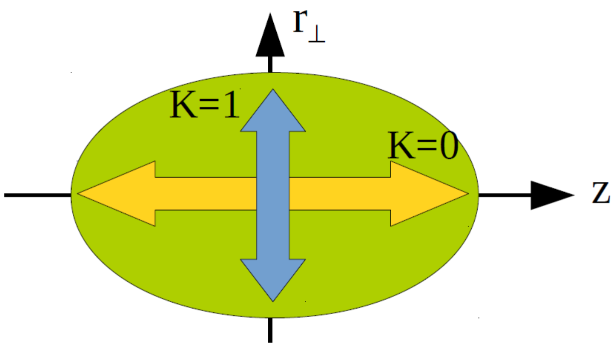
- 9 MeV res. is collective
  no direct relation to cont.

◆ For experimental detection: around zero degrees (Z.H.Yang, et al., PRL, 2014)

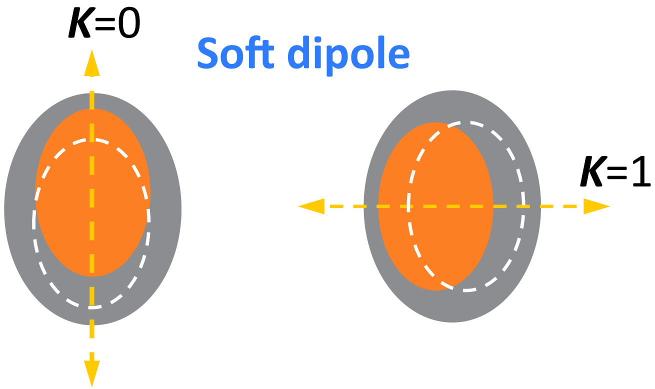
Shape coexistence in ^{40}Mg

- Prolate and oblate coexistence in N=28   From oblate 42Si to prolate 40Mg



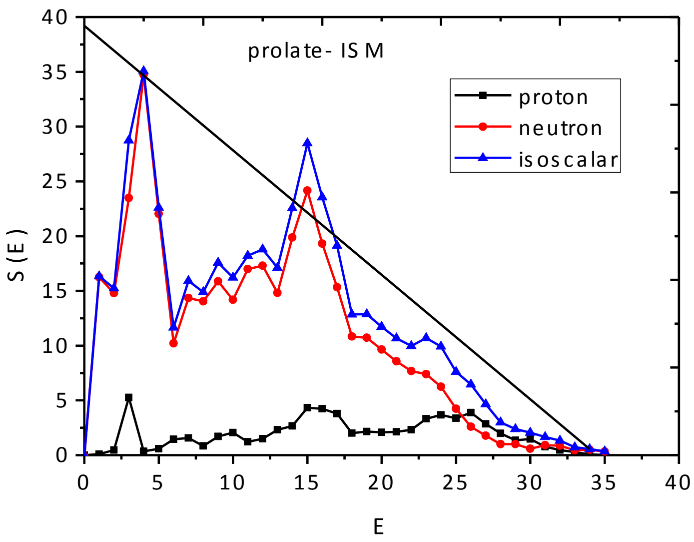


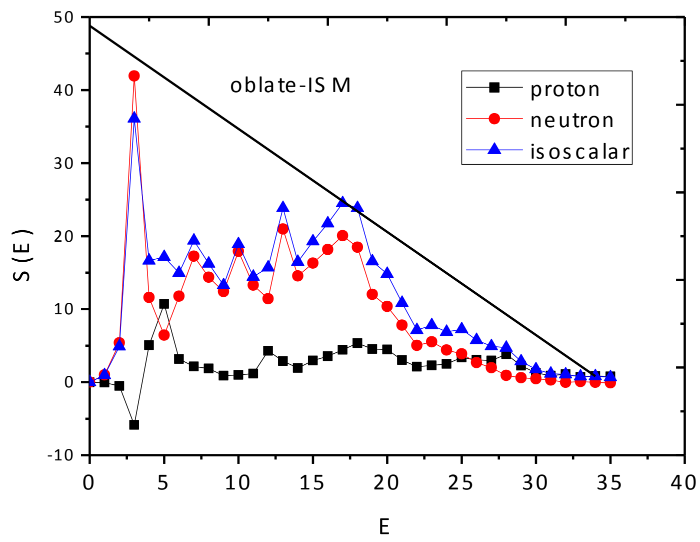
A good case to probe excitations of different deformed halos



Multipole excitations

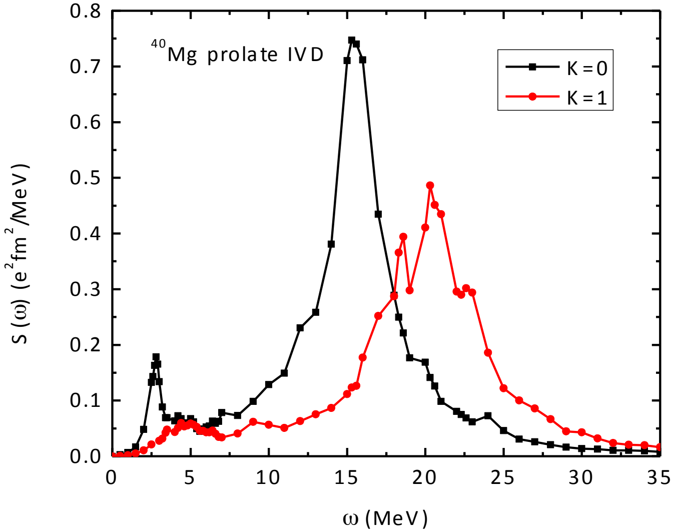
- Isoscalar monopole excitations of prolate and oblate deformations

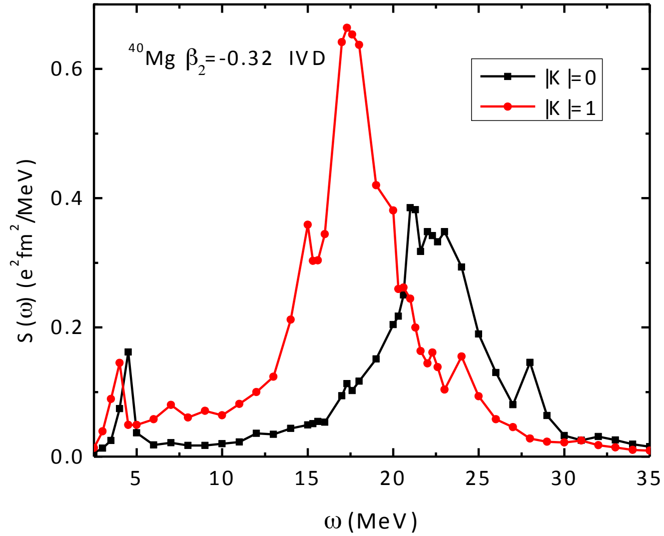


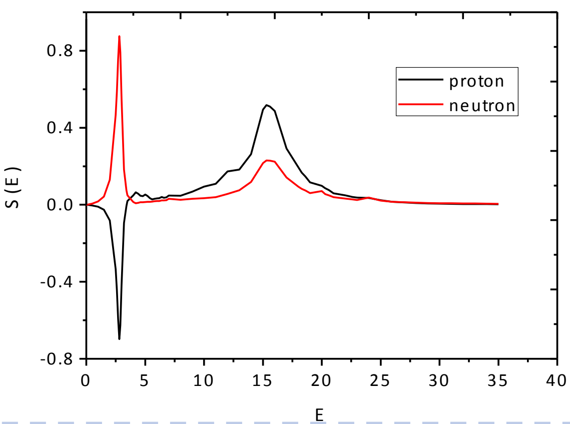


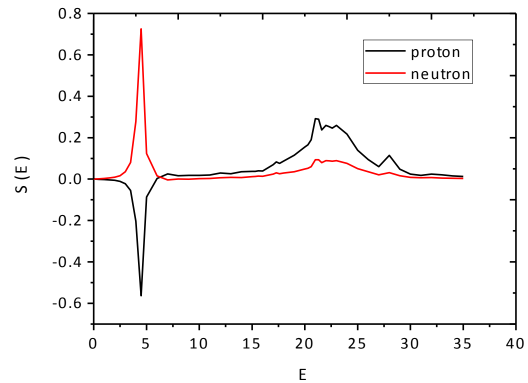
- Remarkable ISM soft modes with different deformations, neutron dominated
- Deformation splitting is not significant in ISM in weakly bound nuclei

- isovector dipole excitations: deformation splitting in pygmy and giant IVD



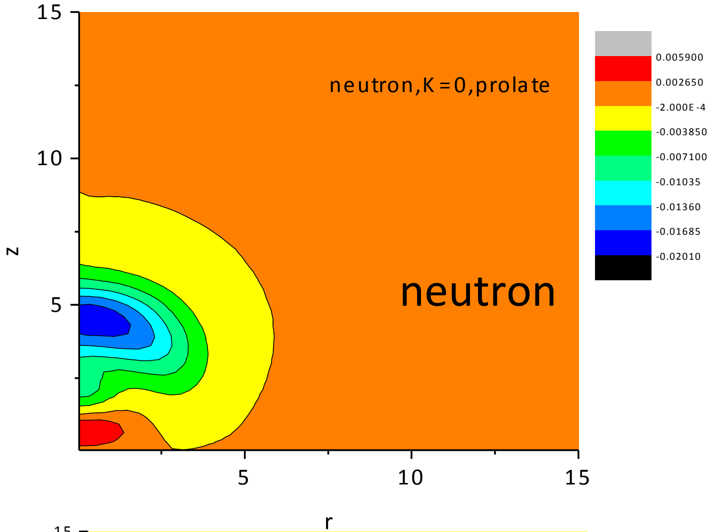


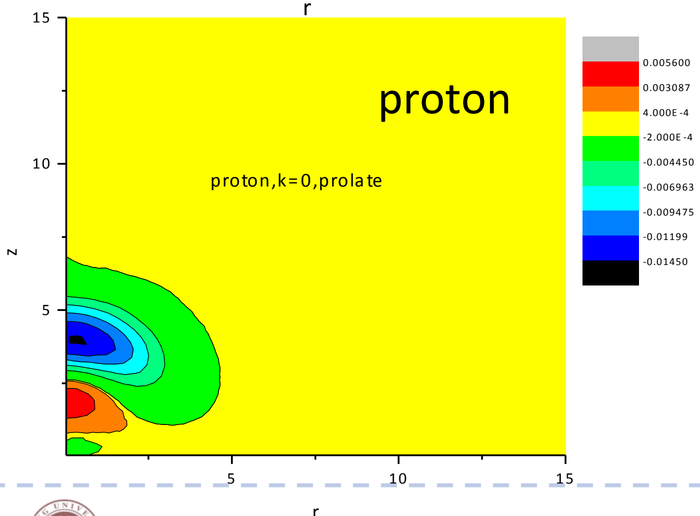




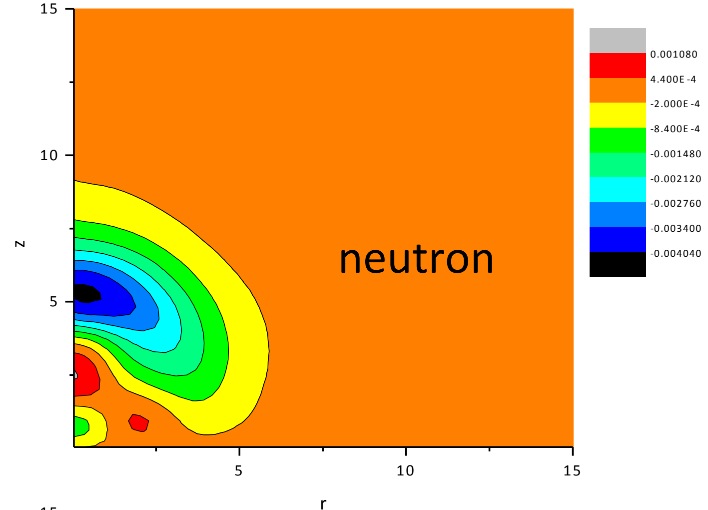
Transition density of IVD

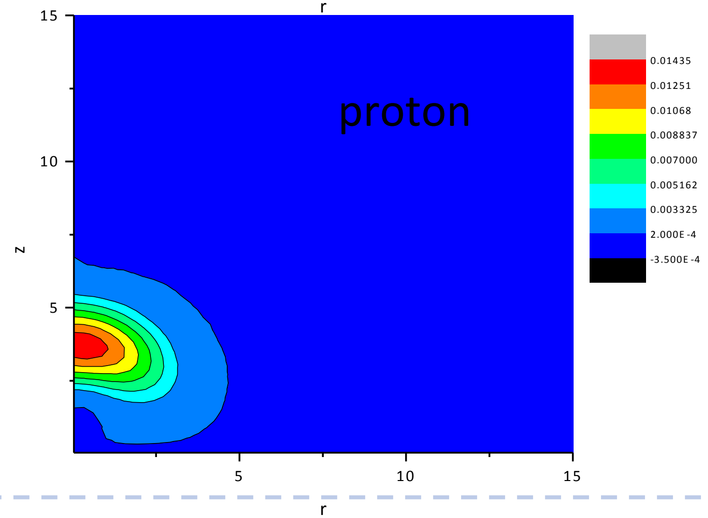
Pygmy IVD (in phase)



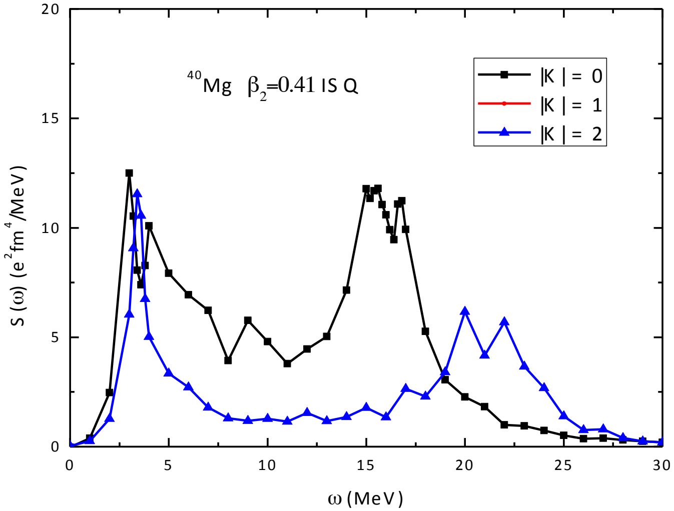


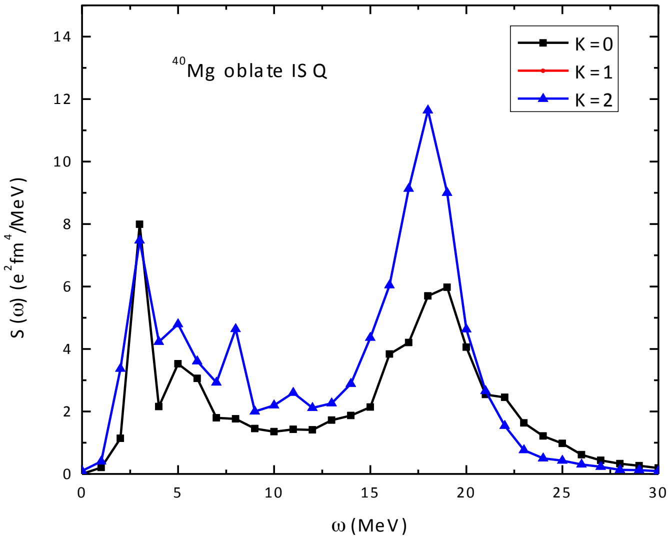
Giant IVD (out phase)

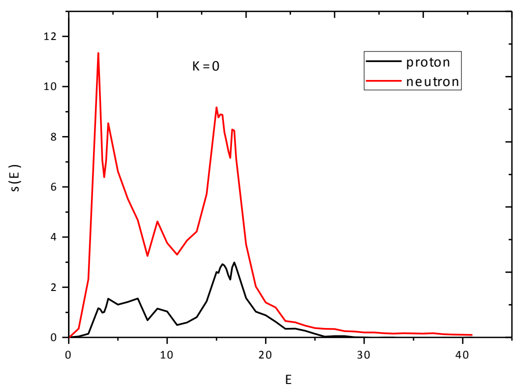


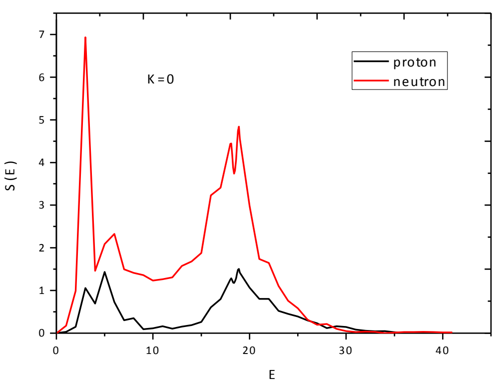


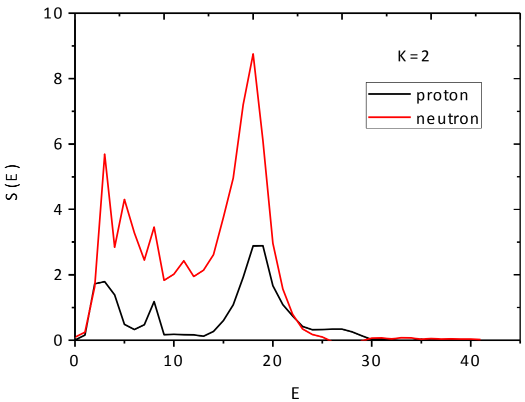
- Isoscalar Quadrupole excitation (spurious in K=1 mode)





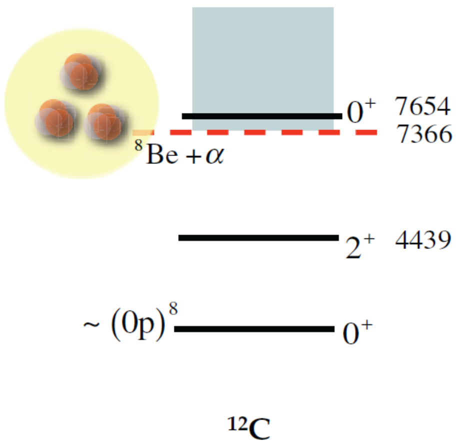




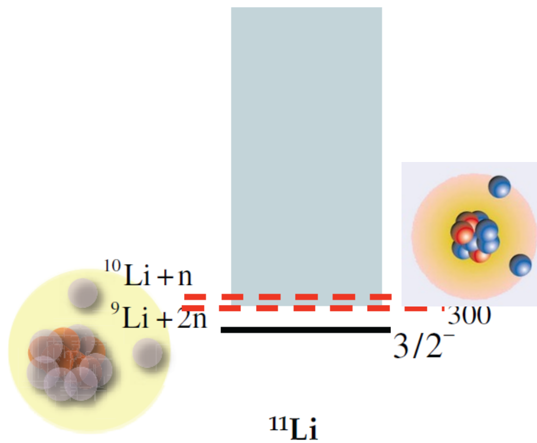


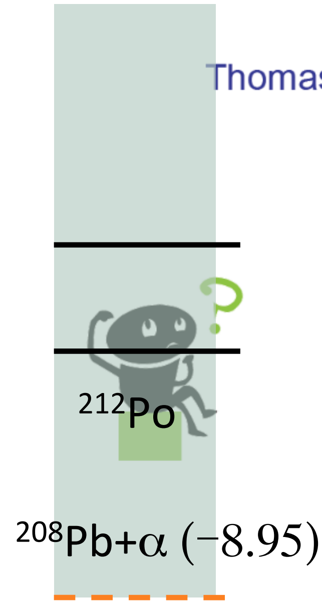
Open problems

α cluster states

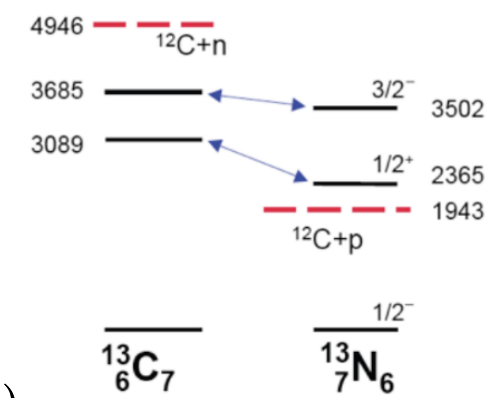


halo states

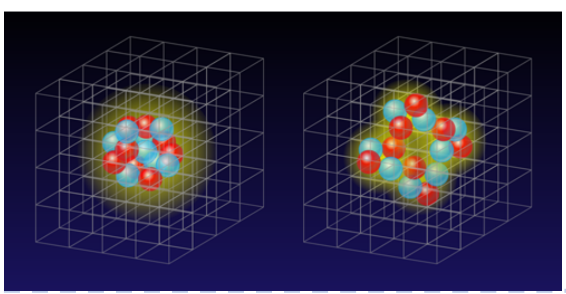




Thomas-Ehrmann shift (1951)



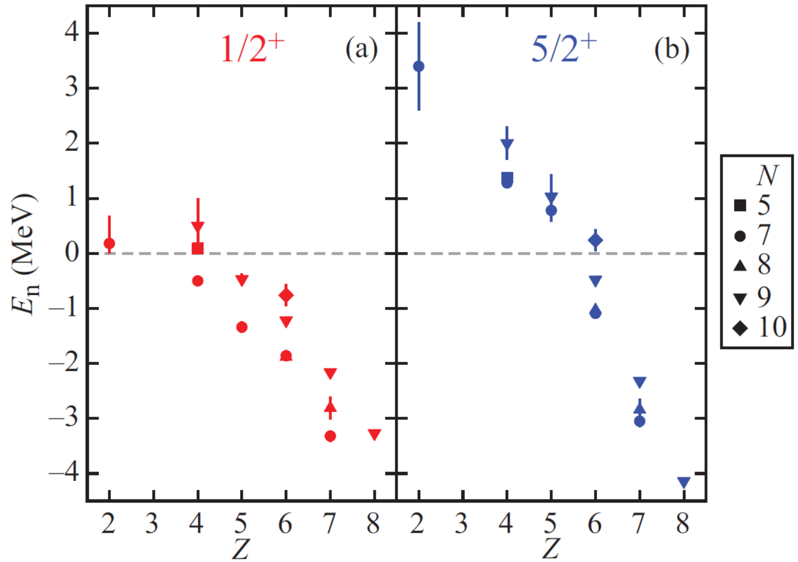
- Continuum and threshold effects
- Localization effects
- Evolution from many-body to few -body



- Lattice effective field theory
- MC shell model
- Gamow shell model

Open problems

- Special s-wave in weakly bound nuclei



Geometry effect influence s-wave

C. R. Hoffman, PRC C 89, 061305(R) 2014

Implications: orbit-dependent interaction is needed;
more halo nuclei than expected

Summary

- Coordinate-space HFB is a suitable tool to explore new exotic halo structures and excitations, with the development of supercomputing
- Various soft modes due to surface vibrations and continuum
- Different mechanisms in pygmy and giant resonances

To be done:

- 3D Continuum FAM-QRPA for multipole excitations
- and more applications for beta decays, pair transfer, collective mass…

Thanks for your attention!

Collaborators: Kai Wang, M. Kortelainen, Yinu Zhang and Furong Xu
And many others for discussions