Int. Conf. on Nuclear Theory in the Supercomputing Era - 2013
Ames
May 16 (13-17), 2013

Monte Carlo Shell Model
and
shape phase transitions in exotic nuclei

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THE UNIVERSITY OF TOKYO

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University of Tokyo / MSU

NSCL

HPCI Strategic Programs for Innovative Research (SPIRE)
Field 5 "The origin of matter and the universe"

We wish a very happy 70th birthday, James

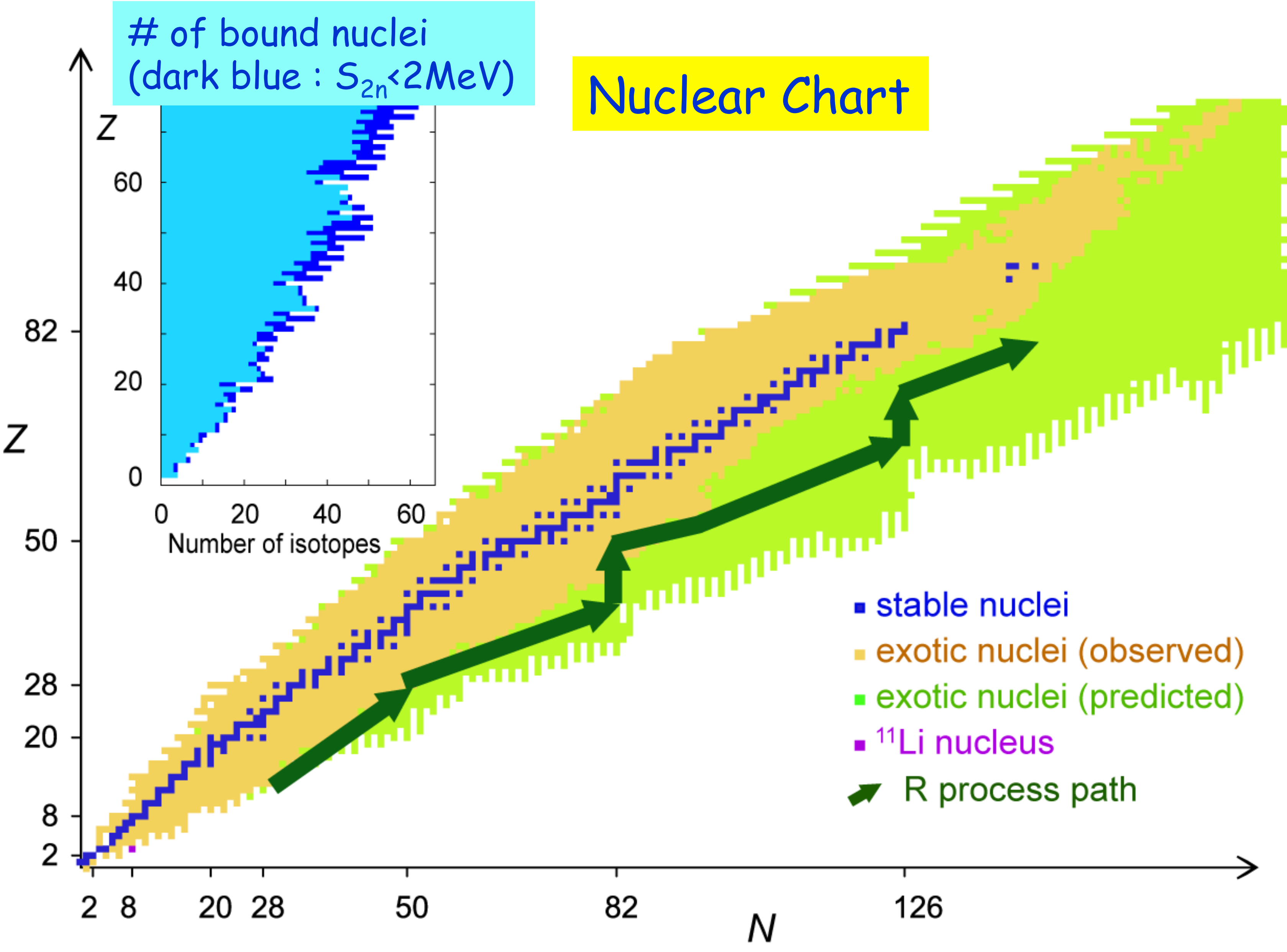
Thank you for our collaborations and also for your help to further developments of computational physics in Japan

Ames, February 2010

Outline

1. Introduction
2. Shape phase transitions in stable nuclei
3. Advanced Monte Carlo Shell Model
4. Shape phase transitions in exotic Ni isotopes
5. Summary

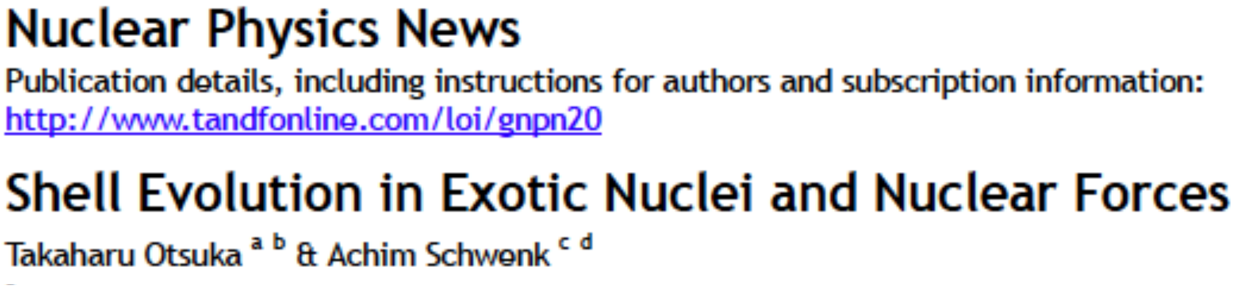
Nuclear Chart



# of bound nuclei
(dark blue : S_{2n}<2MeV)

Theoretical prediction :
Koura *et al*. Prog. Theor. Phys. **113**, (2005) 305.

One of the primary objects can be
to look for paradigm shifts in the understanding of the structure (and reactions) of exotic nuclei
in comparison to the structure of stable nuclei,
i.e., densities, magic numbers, shapes, …

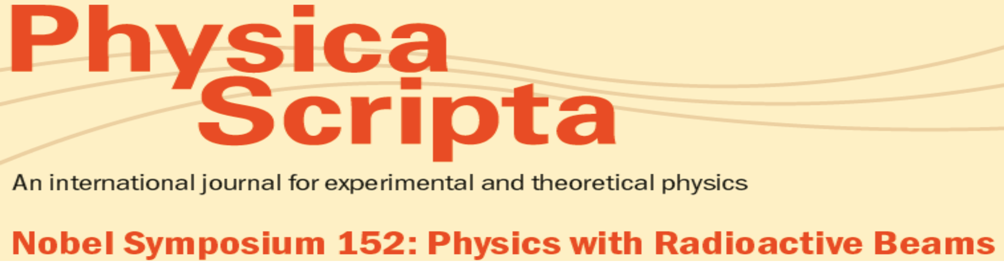


Nuclear Physics News

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gnpn20

Shell Evolution in Exotic Nuclei and Nuclear Forces

Takaharu Otsuka [a] [b] & Achim Schwenk [c] [d]



Physica Scripta

An international journal for experimental and theoretical physics

Nobel Symposium 152: Physics with Radioactive Beams

Exotic nuclei and nuclear forces T. Otsuka

http://iopscience.iop.org/1402-4896/2013/T152/014007

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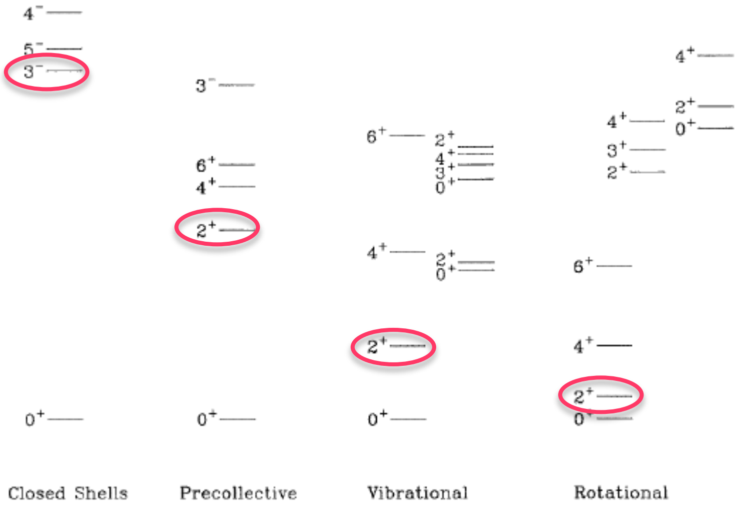
The evolution of nuclear structure: the N_pN_n scheme and related correlations

J. Phys. G: Nucl. Part. Phys. **22** (1996) 1521–1552. Printed in the UK

R F Casten†‡ and N V Zamfir†‡§||



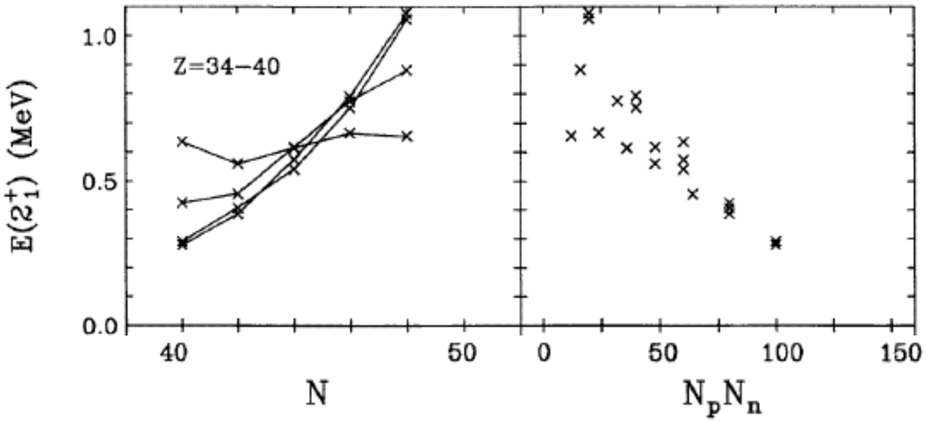


Figure 11. Similar to figure 7 for the $A \sim 80$ region.

N_p : # of protons in one major shell

N_n : # of neutrons in one major shell

N_p x N_n gauges the structure of a given nucleus
to agood extent.

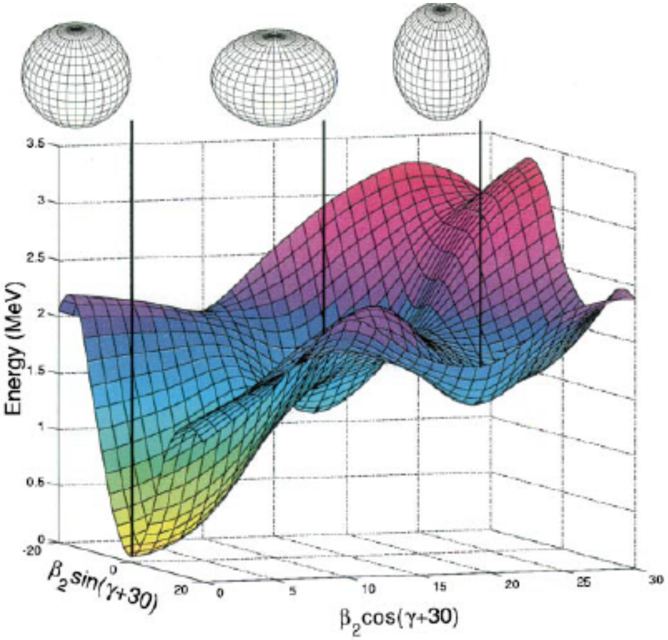
Stable nuclei and their neighbors on the nuclear chart

One nucleus

↓

One shape (sphere, prolate or oblate ellipsoid, etc.)

Excitations occur within the given scheme of shape



Coexistence of different shapes occurs as an exceptional (hence precious and interesting) case.

^{186}Pb

Andreyev *et al.*, Nature **405**, 430 (2000)

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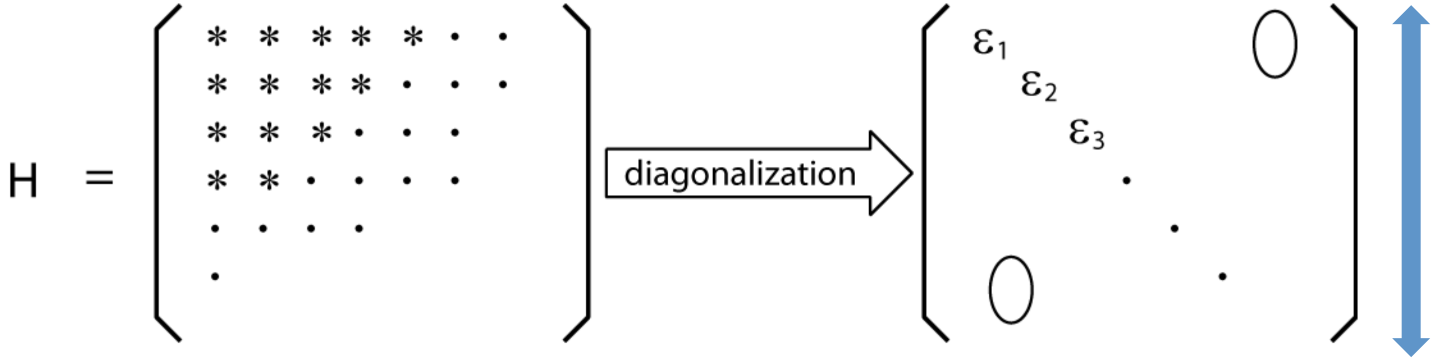
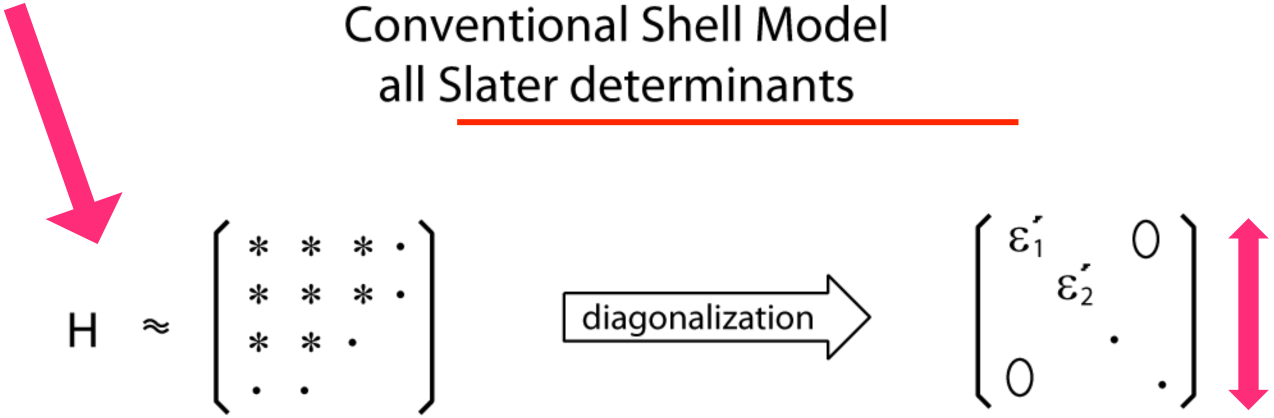
Monte Carlo Shell Model calculations



up to billions

Conventional Shell Model
all Slater determinants

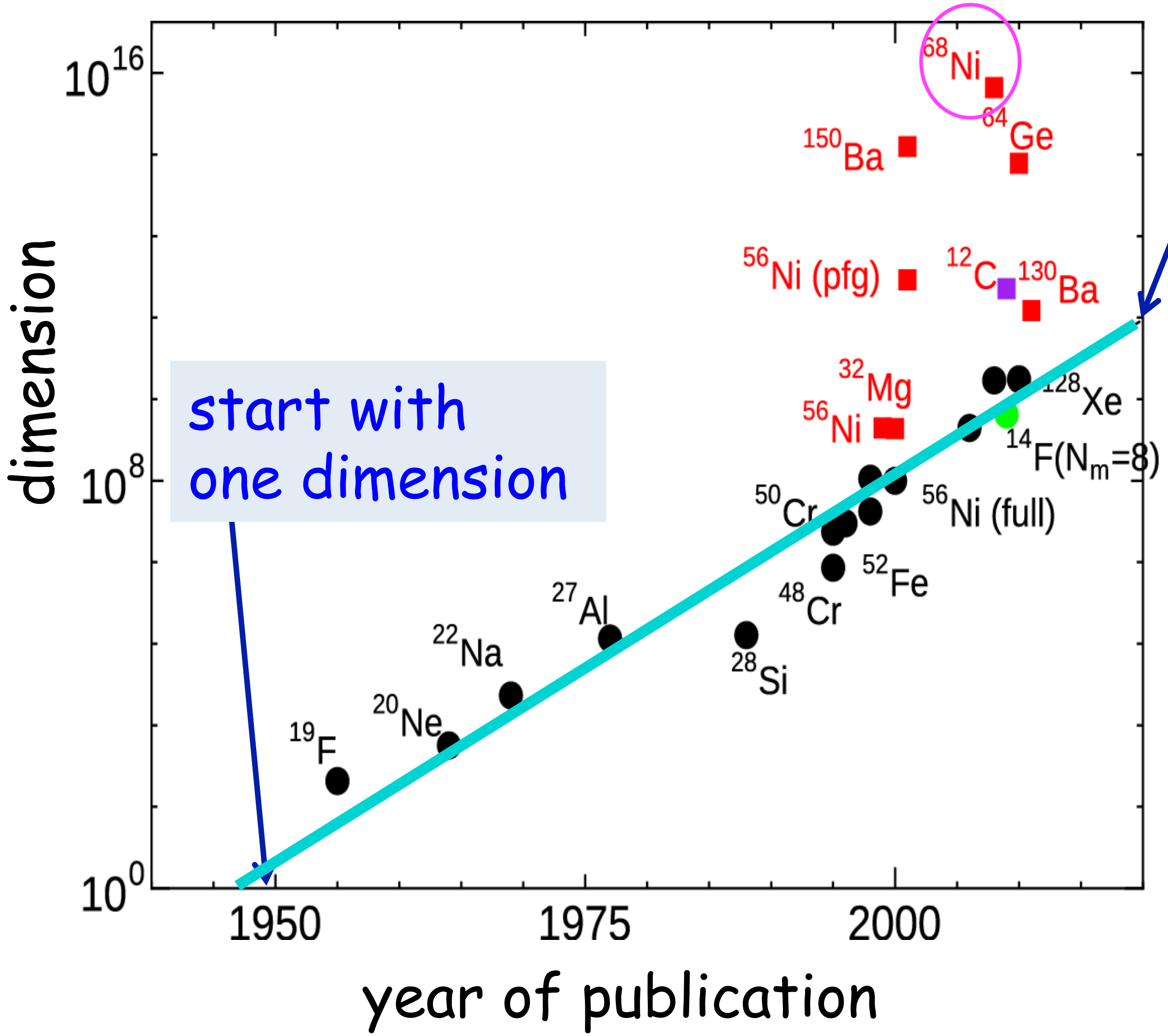


typically ~ 100

Monte Carlo Shell Model
bases important for a specific eigenstate

optimized basis vectors selected by quantum Monte Carlo and by variation-like method

Increase of shell-model dimension



start with
one dimension

Basic trend :
~2 times /year

→1 billion dimension
after 60 years

black, green
circles :
conventional
shell model

red circles :
Monte Carlo
shell model

Note: Importance truncation improves. … Roth's talk

Created by Shimizu

Next generation of Monte Carlo Shell Model

N_B : number of basis vectors (dimension)

N_p : number of (active) particles

N_{sp} : number of single-particle states

$$|\Psi(D)\rangle = \sum_{n=1}^{N_B} c_i P^{J,\Pi} |\phi(D^{(n)})\rangle$$

amplitude

Projection op.

$$|\phi(D^{(n)})\rangle = \prod_{\alpha=1}^{N_p} \underbrace{\left(\sum_{i=1}^{N_{sp}} a_i^{\dagger} D_{i\alpha}^{(n)}\right)}_{\text{Deformed single-particle state}} |-\rangle$$

N-th basis vector (Slater determinant)

$$E(D) = \langle \Psi(D) | H | \Psi(D) \rangle$$

Minimize *E(D)* as a function of *D* utilizing qMC and conjugate gradient methods

Step 1 : quantum Monte Carlo type method

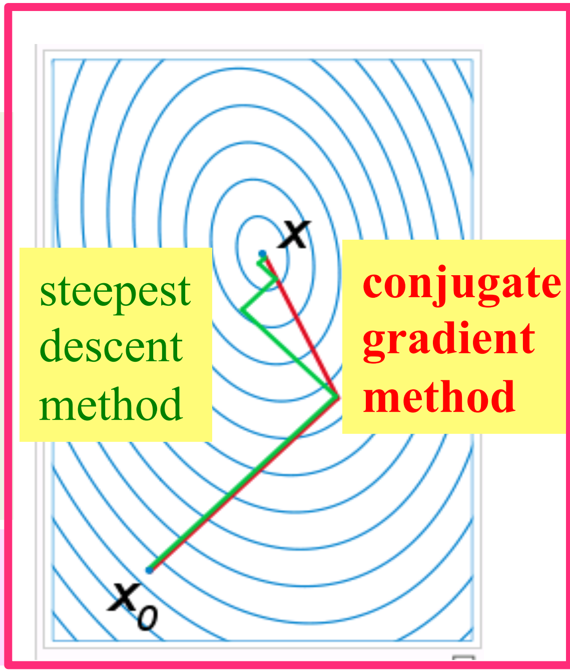
→ candidates of n-th basis vector (σ: set of random numbers)

$$|\phi(\sigma)\rangle = \prod e^{\Delta\beta \cdot h(\sigma)} \cdot |\phi^{(0)}\rangle$$

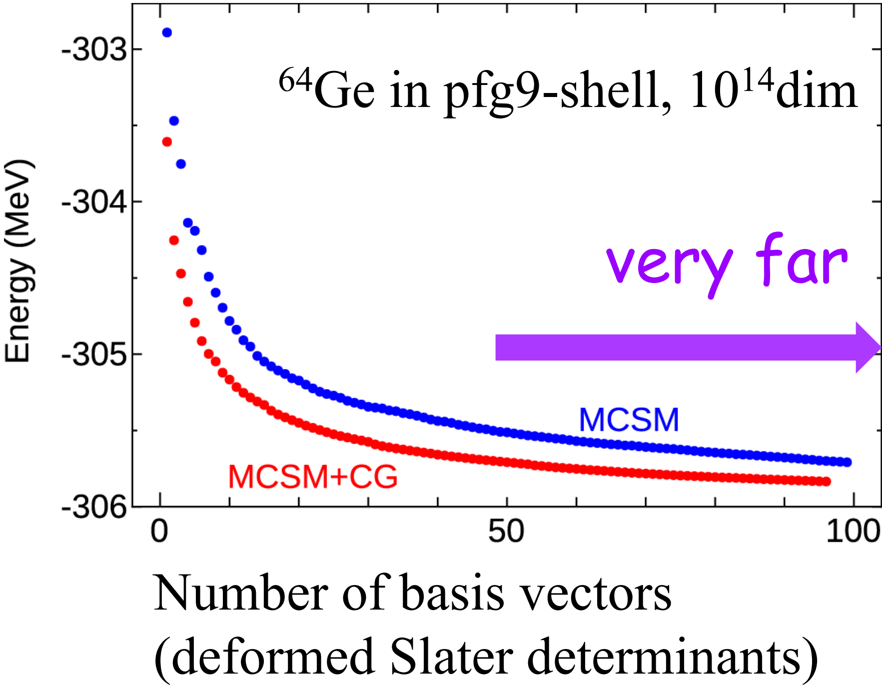
"σ" can be represented by matrix D

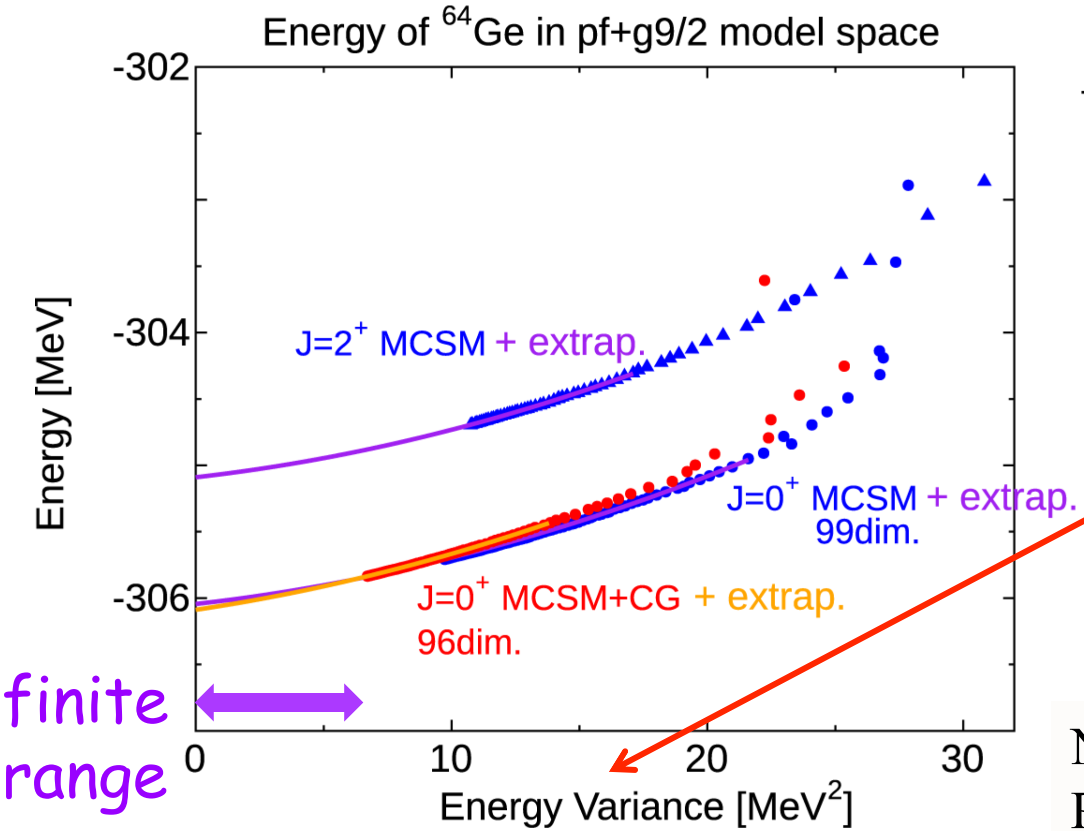
Select the one with the lowest *E(D)*

Step 2 : polish *D* by means of the conjugate gradient method "variationally".



Extrapolation by Energy Variance





Variance : $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$

$$\langle H \rangle = E_0 + a\langle \Delta H^2 \rangle + b\langle \Delta H^2 \rangle^2 + \dots$$

N. Shimizu, et al.,
Phys. Rev. C **82,** 061305(R) (2010).

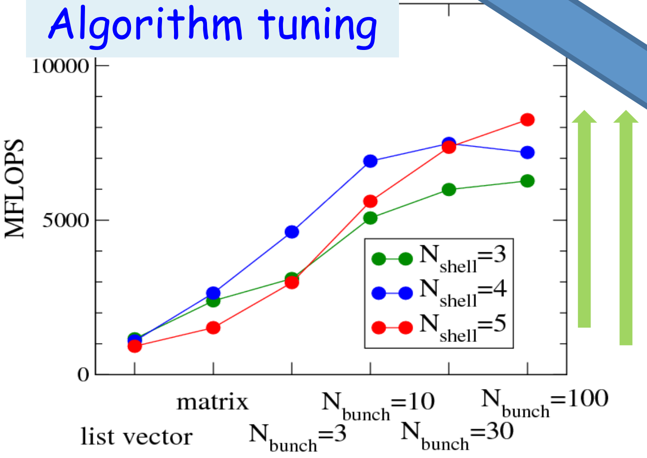
Combining all improvements

T. Otsuka, M. Honma, T. Mizusaki, N. Shimizu, and Y. Utsuno, Prog. Part. Nucl. Phys. **47**, 319 (2001).

PC cluster
100CPU parallel

2001

Algorithm tuning

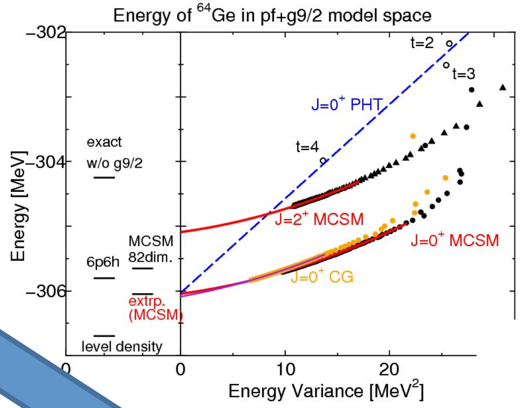


Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe,
Comp. Phys. Com., 184, 102-108 (2013)

8 times faster at maximum

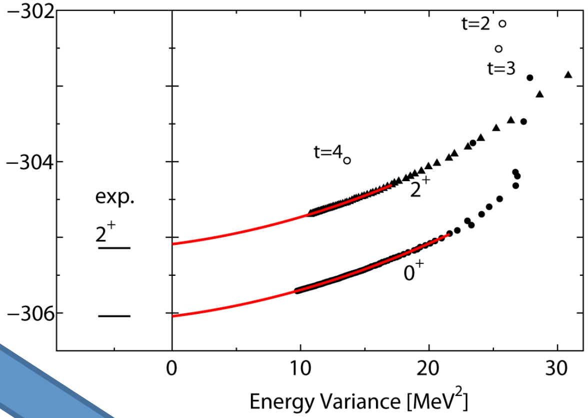
Conjugate Gradient method

N. Shimizu *et al*, Phys. Rev C 85 054301 (2012)

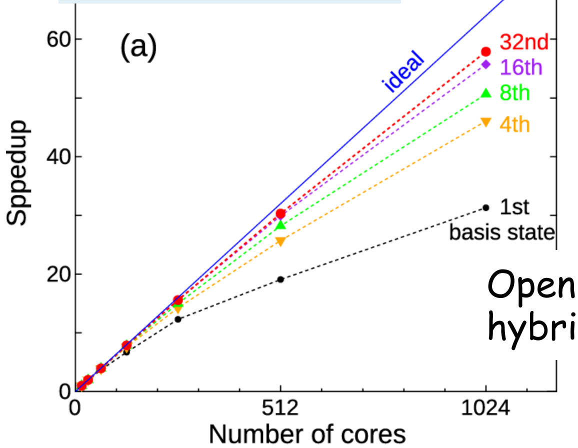


N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe, and M. Honma, Phys. Rev. C **82**, 061305(R) (2010).

Variance extrapolation + reordering technique



Parallel efficiency



OpenMP+MPI
hybrid parallel

N. Shimizu *et al.*,
Prog. Theor. Exp. Phys. 2012

SPARC64 VIIIfx
705,024 cores

K computer

Major computational work in MCSM :
Projection of deformed Slater determinants
(many-body basis vectors) onto good J and parity

Rotation with three Euler angles numerically
-> about 50,000 mesh points of the angles

K computer (in Kobe)
10 peta flops machine
(3rd fastest)

HPCI Strategic Programs for Innovative Research (SPIRE)
Field 5 "The origin of matter and the universe"

One of 4 groups is for nuclear structure (mainly MCSM)

Example : 8^+ ^{68}Ni 7680 cpu core x 14 h

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Ni and neighboring nuclei

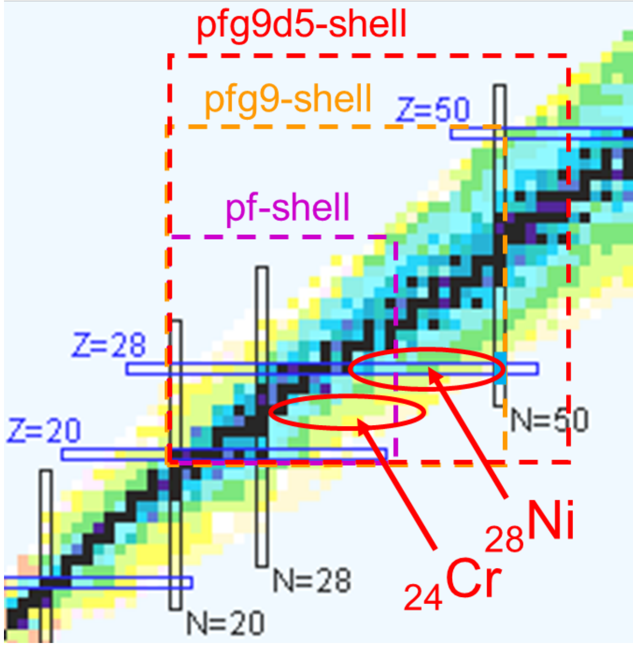
Configuration space

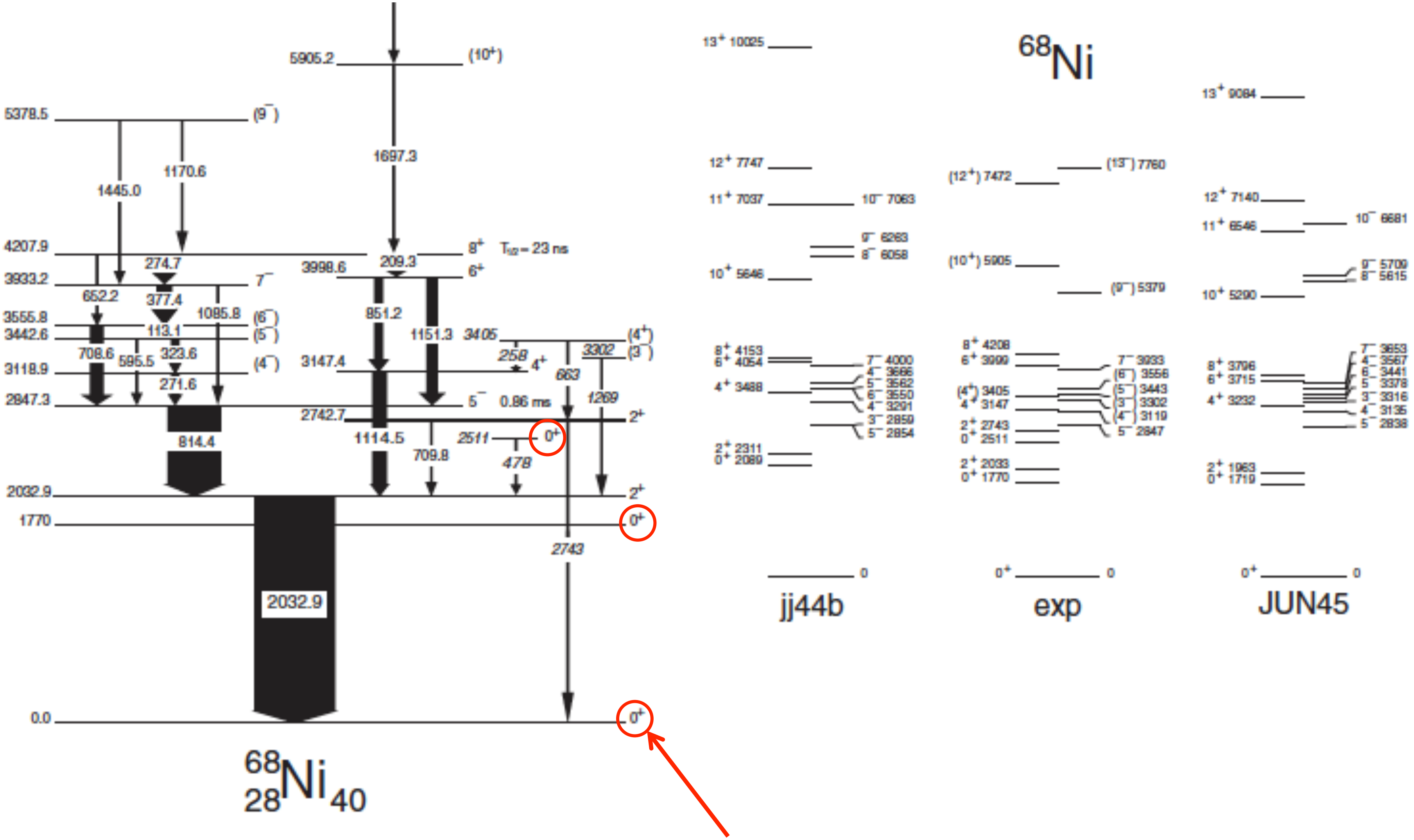
- pfg9d5-shell ($f_{7/2}$, $p_{3/2}$, $f_{5/2}$, $p_{1/2}$, $g_{9/2}$, $d_{5/2}$)
  → large Hilbert space (5 x 10^{15} dim. for ^{68}Ni) accessible by MCSM

Effective interaction : based on A3DA interaction by Honma

- Two-body matrix elements (TBME) consist of microscopic and empirical ints.
  - GXPF1A (pf-shell)
  - JUN45 (some of f5pg9)
  - G-matrix (others)

- Revision for single particle energy (SPE) and monopole part of TBME

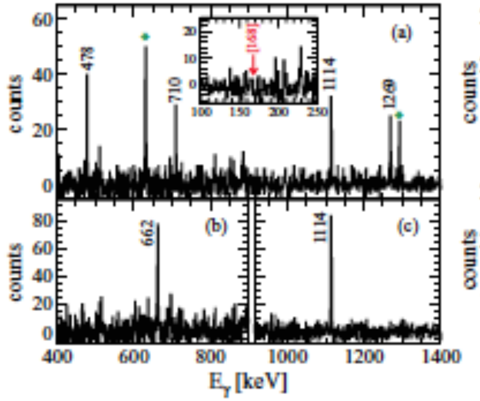


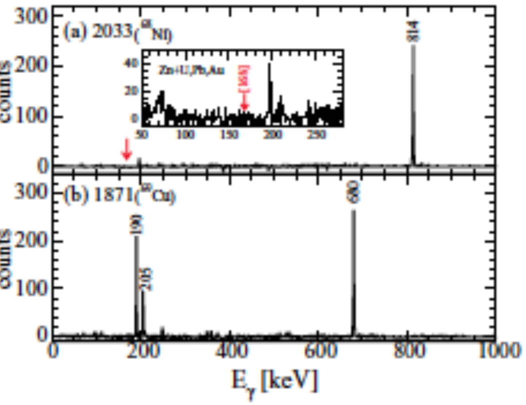


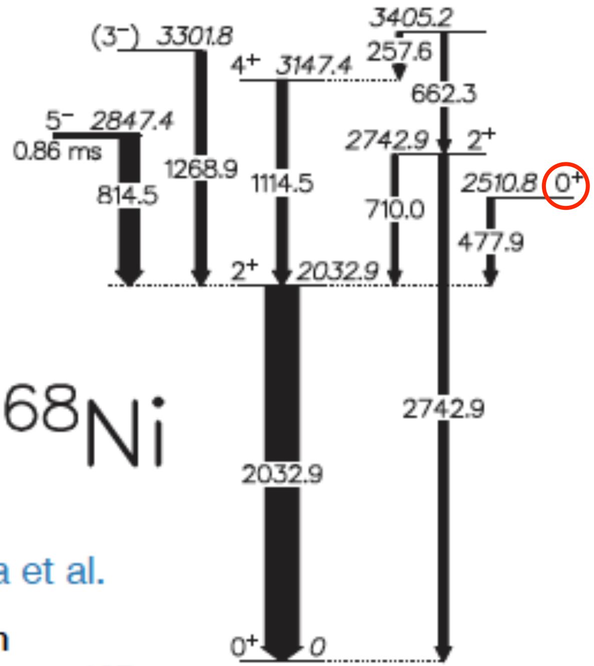
PHYSICAL REVIEW C **67**, 044314 (2003)

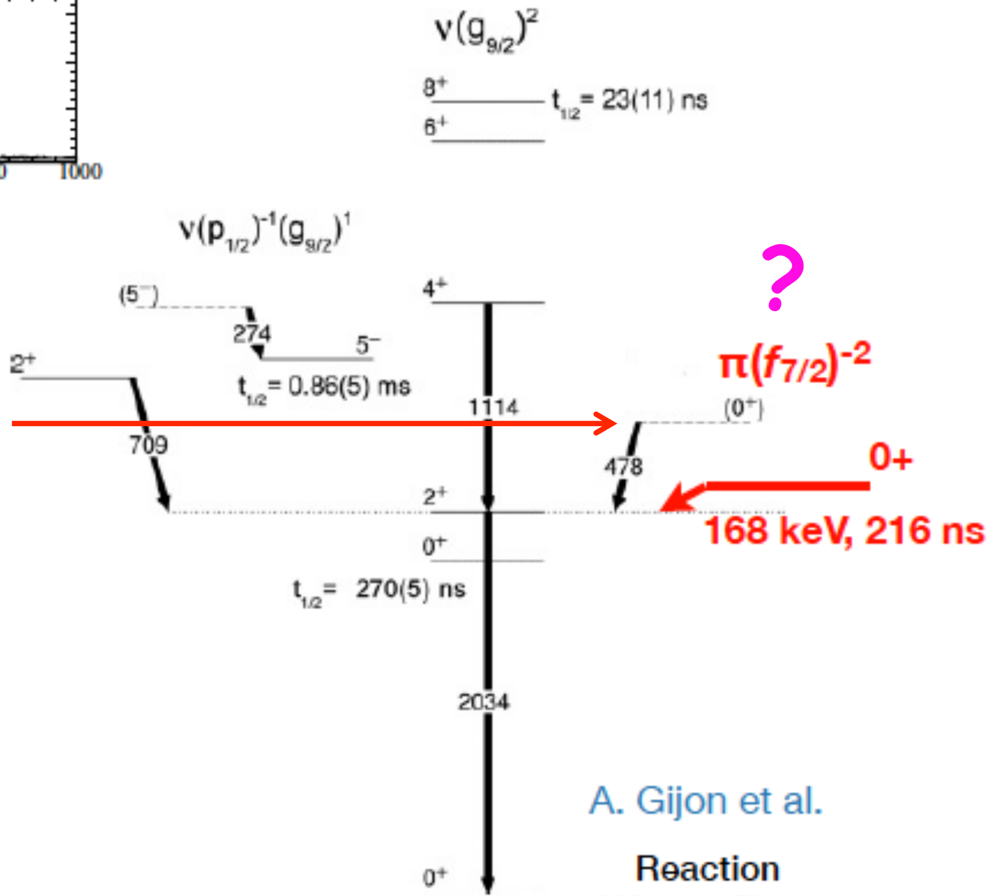
How magic is the magic ^{68}Ni nucleus?

K. Langanke,[1,2] J. Terasaki,[2,3,4] F. Nowacki,[5] D. J. Dean,[2] and W. Nazarewicz[2,3,6]









C.J. Chiara et al.

Reaction

^{70}Zn + ^{238}U, ^{208}Pb, ^{197}Au

A. Gijon et al.

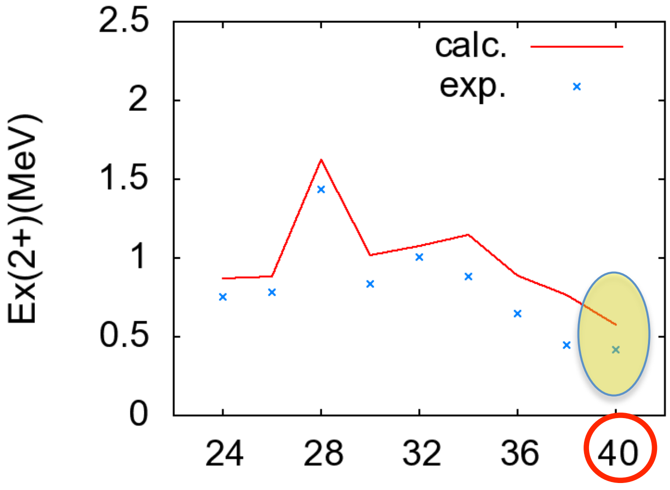
Reaction

^{238}U + ^{70}Zn

Results of Cr and Ni

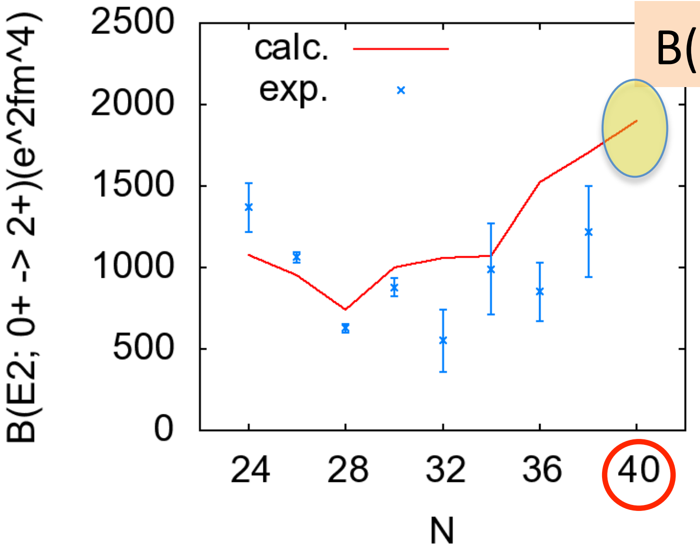
$_{24}$Cr isotopes

- N=40 gap is small



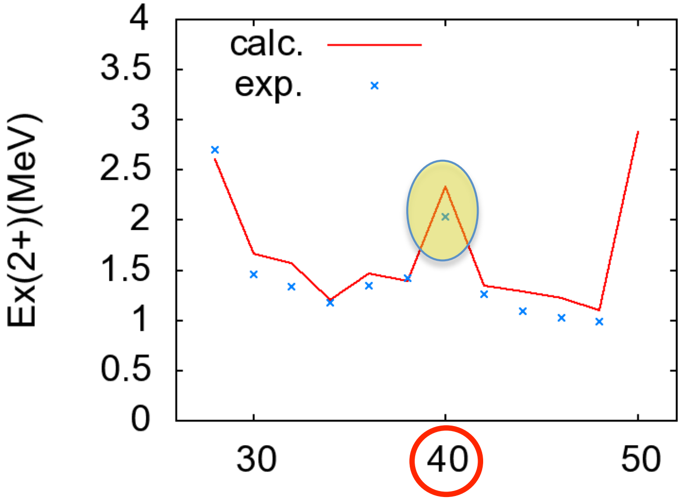
2^+ level

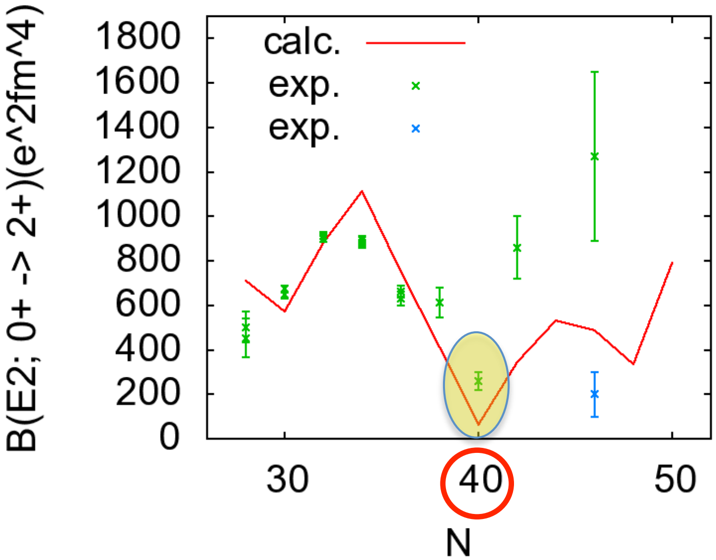
$B(E2; 0^+ \longrightarrow 2^+)$



$_{28}$Ni isotopes

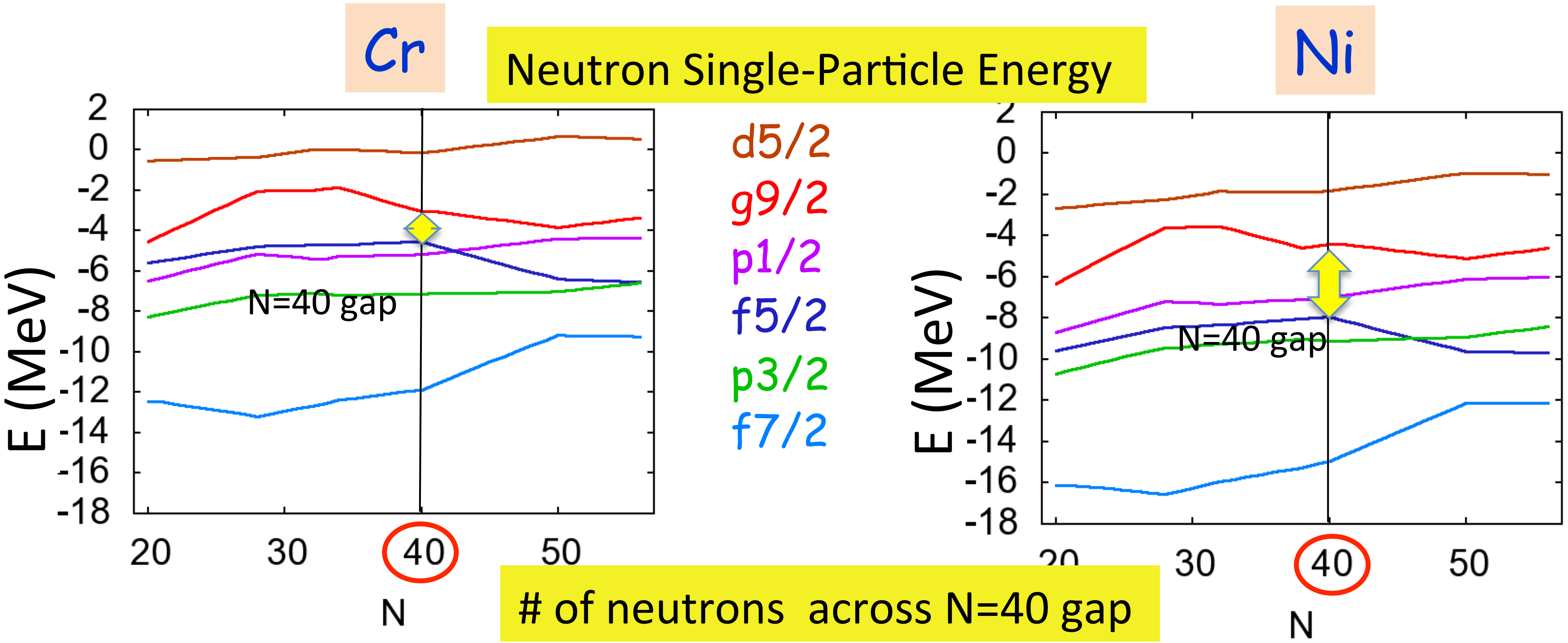
- N=40 gap is large



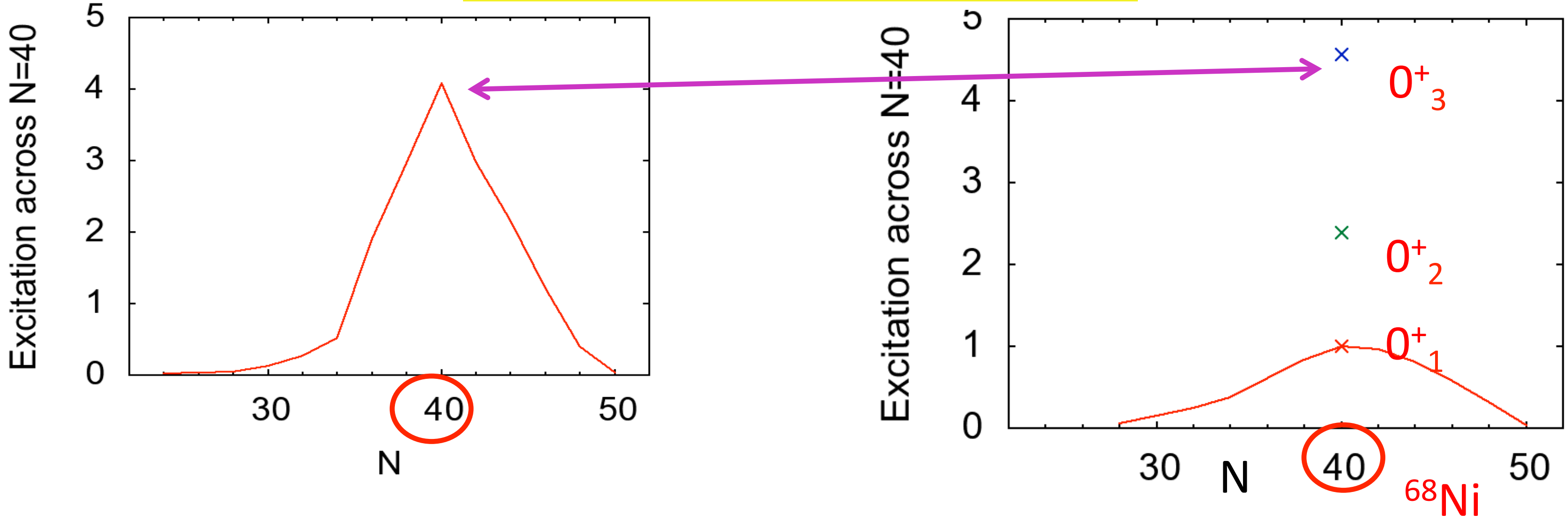


N=40 gap and excitations across it in Cr and Ni isotopes

Neutron Single-Particle Energy



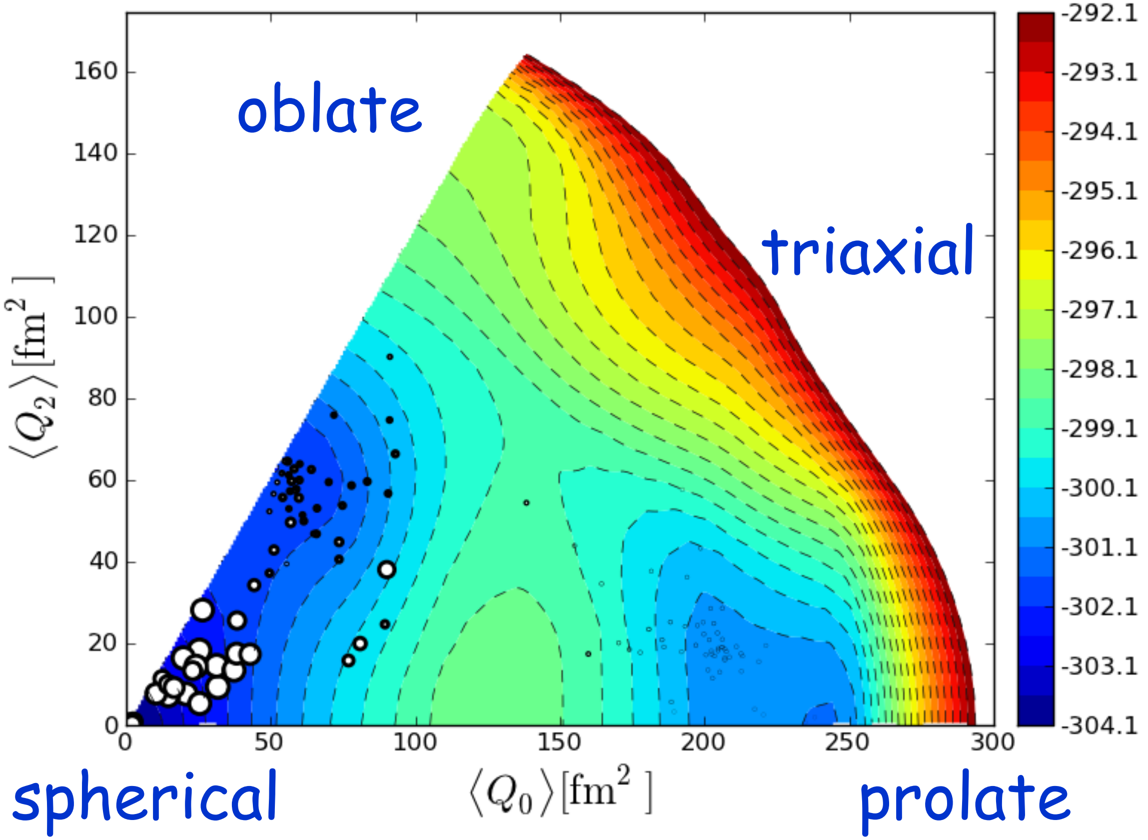
# of neutrons across N=40 gap



MCSM basis vectors on Potential Energy Surface

- PES is calculated by CHF
- Location of circle : quadrupole deformation of unprojected MCSM basis vectors
- Area of circle : overlap probability between each projected basis and eigen wave function

0^+_1 state of ^{68}Ni



Next generation of Monte Carlo Shell Model

N_B : number of basis vectors (dimension)

N_p : number of (active) particles

N_{sp} : number of single-particle states

$$\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} c_i P^{J,\Pi} \left|\phi(D^{(n)})\right\rangle$$

amplitude

Projection op.

$$\left|\phi(D^{(n)})\right\rangle = \prod_{\alpha=1}^{N_p} \underbrace{\left(\sum_{i=1}^{N_{sp}} a_i^{\dagger} D_{i\alpha}^{(n)} \right)}_{\text{Deformed single-particle state}} \left|-\right\rangle$$

N-th basis vector (Slater determinant)

$$E(D) = \left\langle \Psi(D) \middle| H \middle| \Psi(D) \right\rangle$$

Minimize *E(D)* as a function of *D* utilizing qMC and conjugate gradient methods

Step 1 : quantum Monte Carlo type method

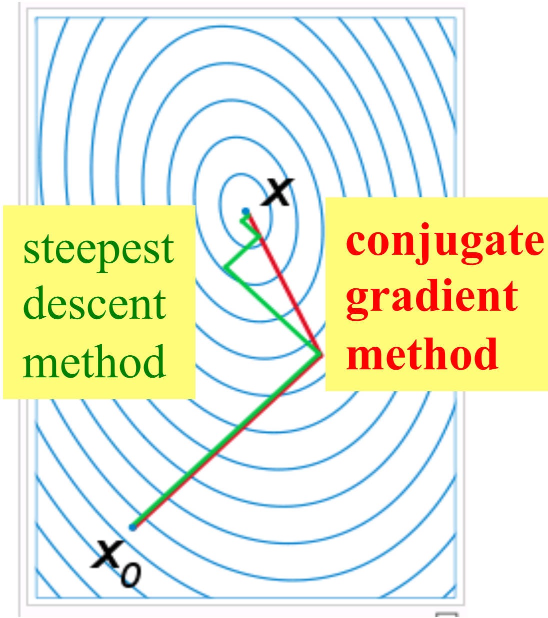
→ candidates of n-th basis vector (σ : set of random numbers)

$$\left|\phi(\sigma)\right\rangle = \prod e^{\Delta\beta \cdot h(\sigma)} \cdot \left|\phi^{(0)}\right\rangle$$

" σ " can be represented by matrix D

Select the one with the lowest *E(D)*

Step 2 : polish *D* by means of the conjugate gradient method "variationally".



^{68}Ni 0$^+$ states ⇔ different shapes

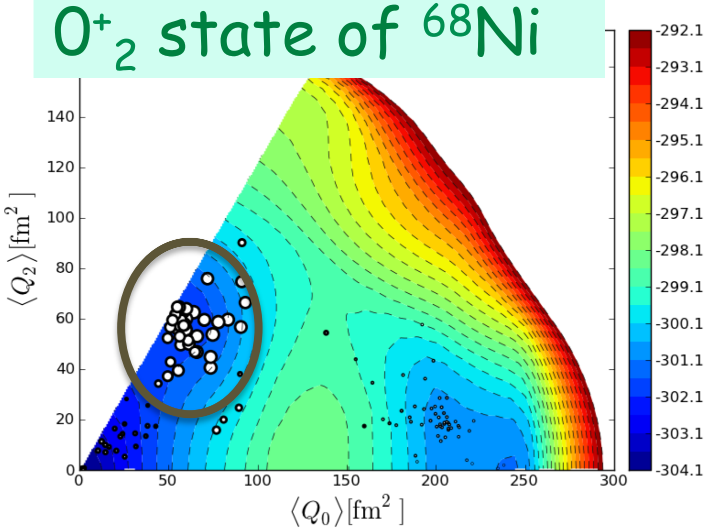
- ^{68}Ni 0^+_1 - 0^+_3 states are comprised mainly of basis vectors generated in

  0^+_1 : spherical

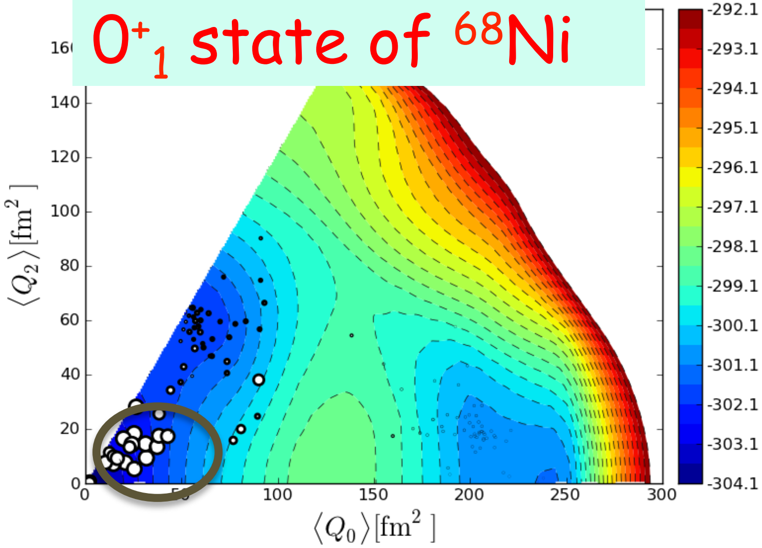
  0^+_2 : oblate

  0^+_3 : prolate

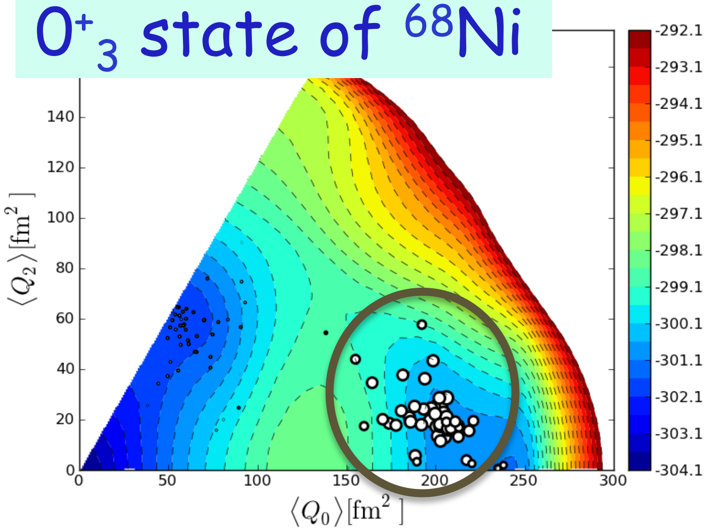
0^+_2 state of ^{68}Ni



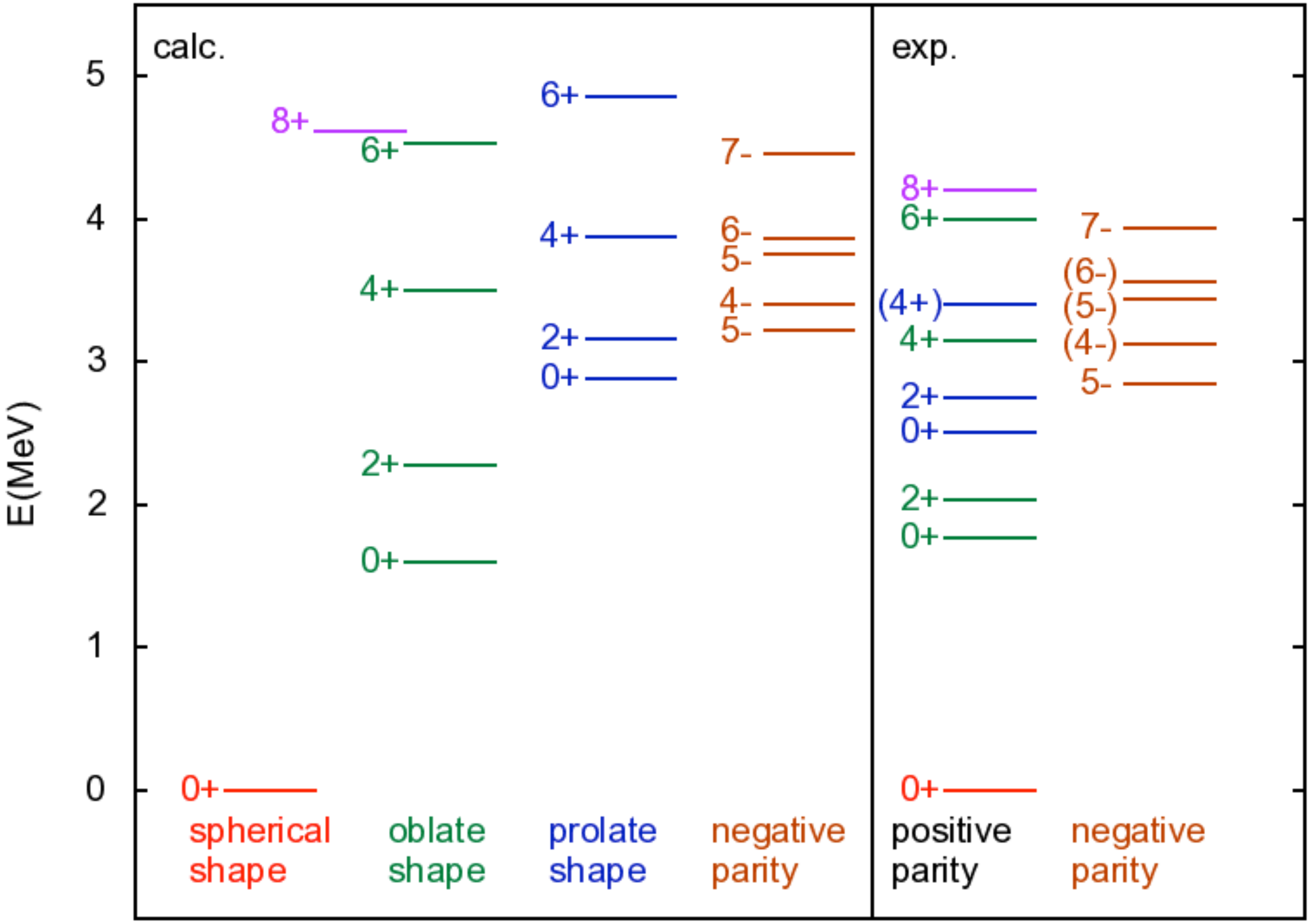
0^+_1 state of ^{68}Ni



0^+_3 state of ^{68}Ni



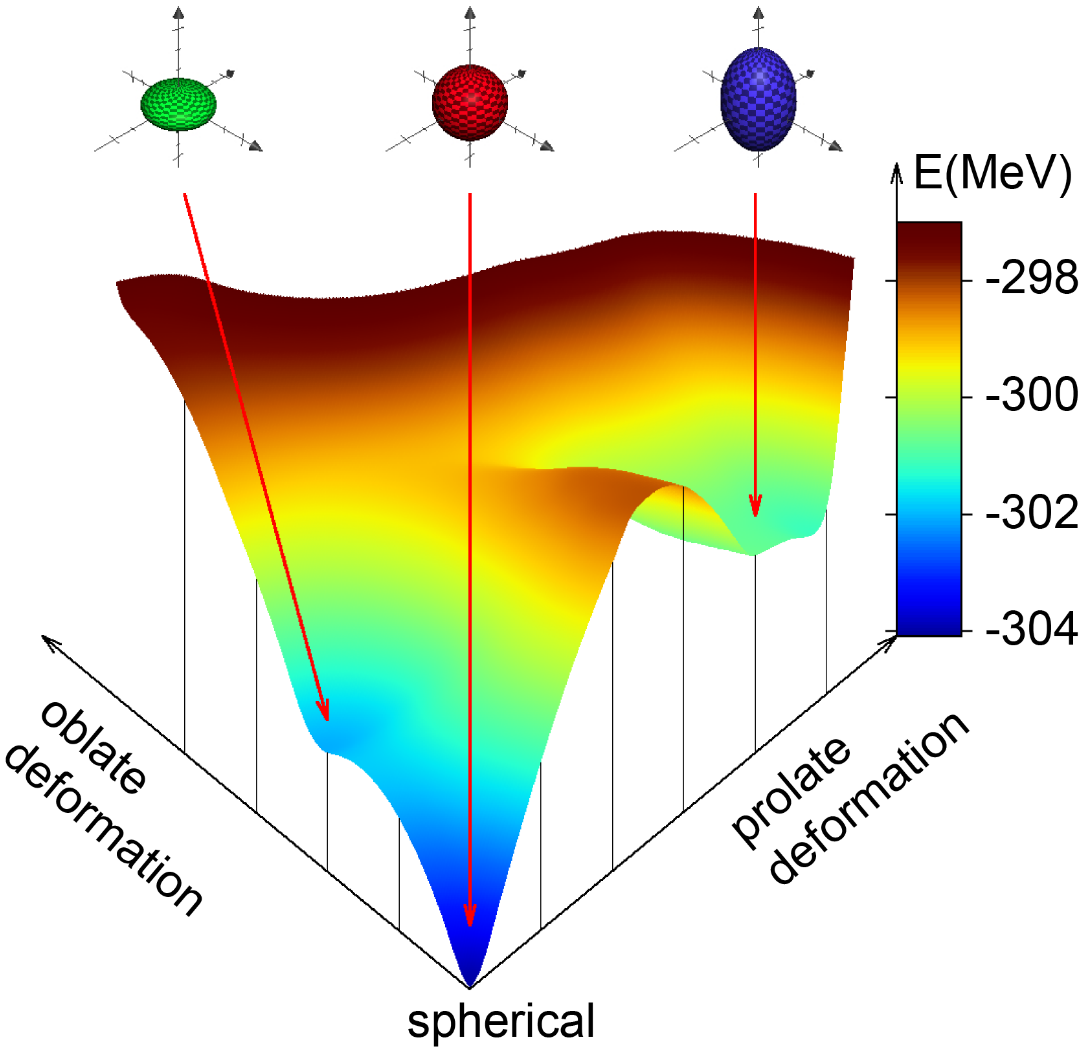
Rich structure of ^{68}Ni



Neutron excitation across N=40: ~1.0 ~2.4 ~4.5 <- order parameter

deformation parameter (2^+) $\beta \sim -0.2$ $\beta \sim 0.4$

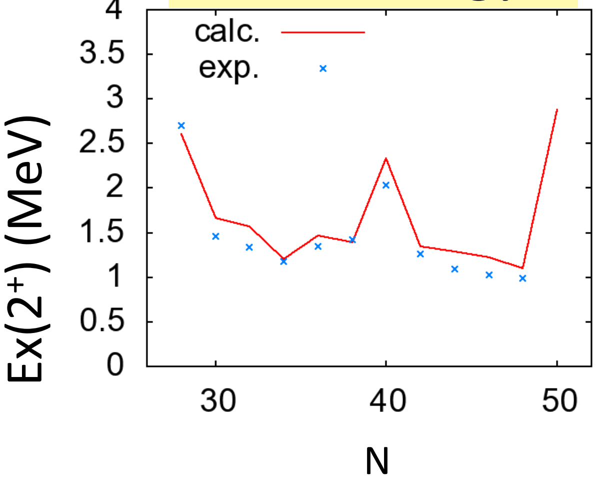
In short, ^{68}Ni looks like …



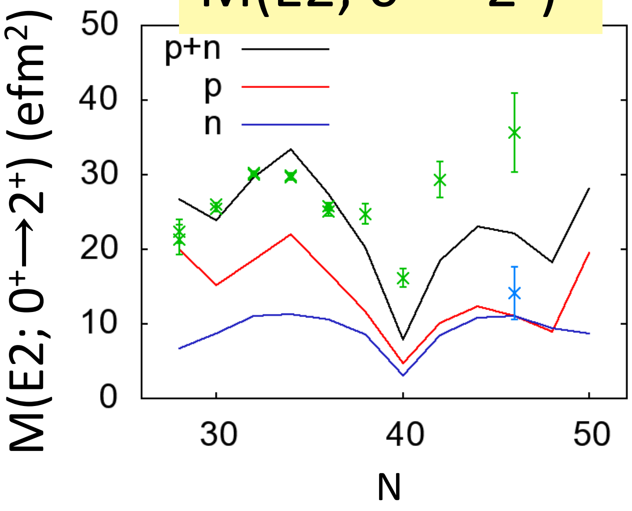
(Lost) Double magicity of ^{56,68,78}Ni

- 2^+ energy and B(E2) are large for ^{56}Ni, ^{78}Ni
- Larger fluctuation of the shape for ^{56}Ni, ^{78}Ni than for ^{68}Ni

2^+ Ex. Energy



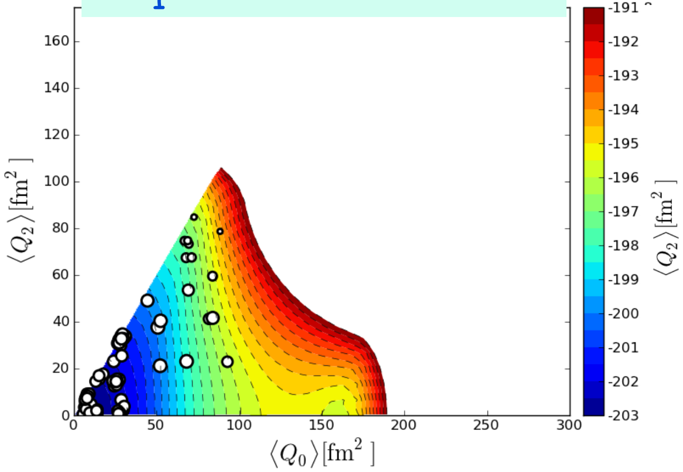
M(E2; $0^+ \longrightarrow 2^+$)



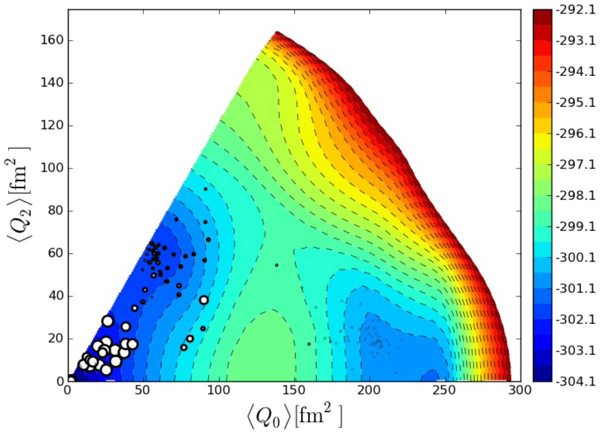
× B. Pritychenko, et al., arXiv:1102.3365v2 (2011)

× de Angelis, private communication

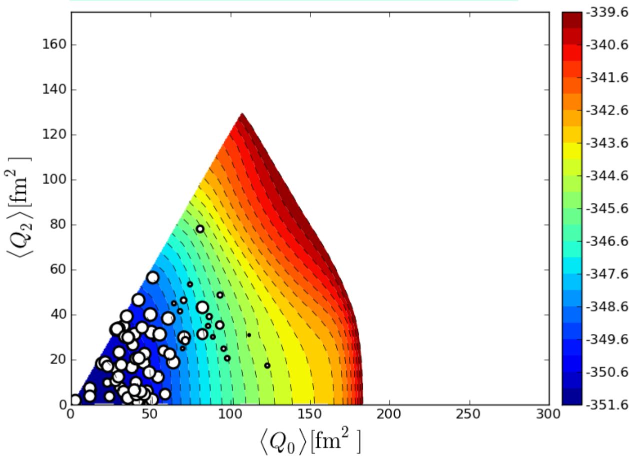
0^+_1 state of ^{56}Ni



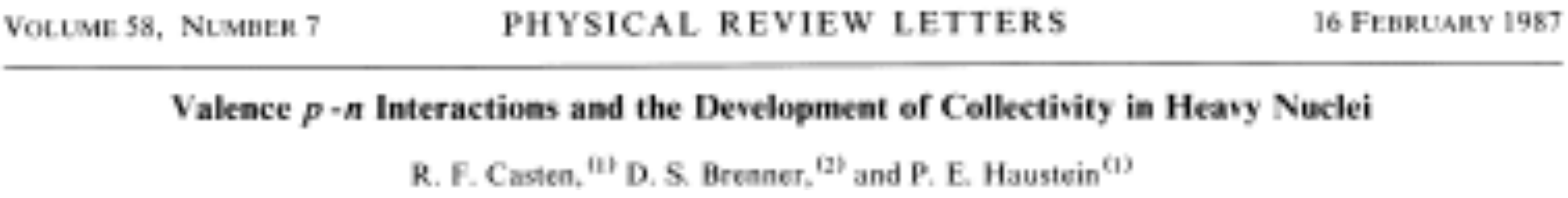
0^+_1 state of ^{68}Ni



0^+_1 state of ^{78}Ni



N_pN_n systematics



VOLUME 58, NUMBER 7 PHYSICAL REVIEW LETTERS 16 FEBRUARY 1987

Valence *p*-*n* Interactions and the Development of Collectivity in Heavy Nuclei

R. F. Casten,(1) D. S. Brenner,(2) and P. E. Haustein(1)

$^{68}_{28}\mathrm{Ni}_{40}$

	ΔN_p	ΔN_n	$N_p N_n$	$N_p + N_n$	$P = N_p N_n/(N_p + N_n)$
0^+_1	0.21	1.00	0.84	2.42	0.35
0^+_2	0.72	2.39	6.88	6.22	1.11
0^+_3	2.57	4.56	46.88	14.26	3.29

$N_p = 2\Delta N_p$

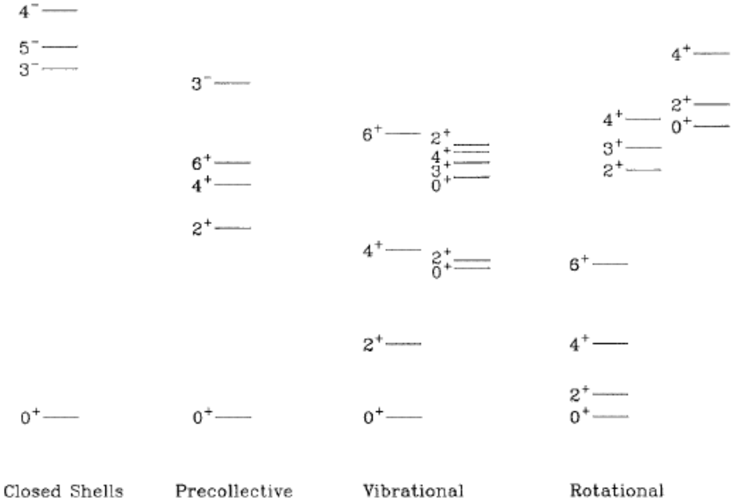
$N_n = 2\Delta N_n$

particles + holes

The evolution of nuclear structure: the N_pN_n scheme and related correlations

J. Phys. G: Nucl. Part. Phys. **22** (1996) 1521–1552. Printed in the UK

R F Casten†‡ and N V Zamfir†‡§||



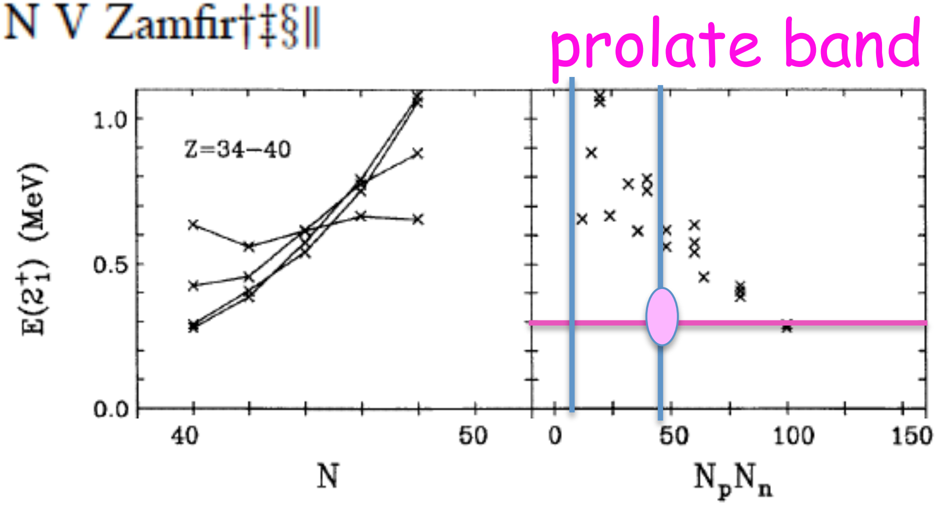


Figure 11. Similar to figure 7 for the $A \sim 80$ region.

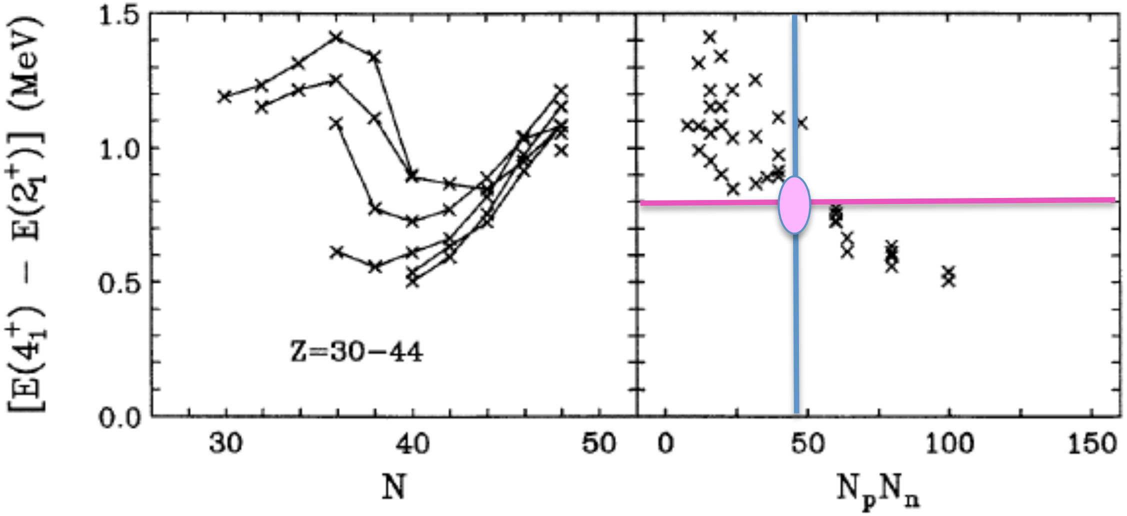
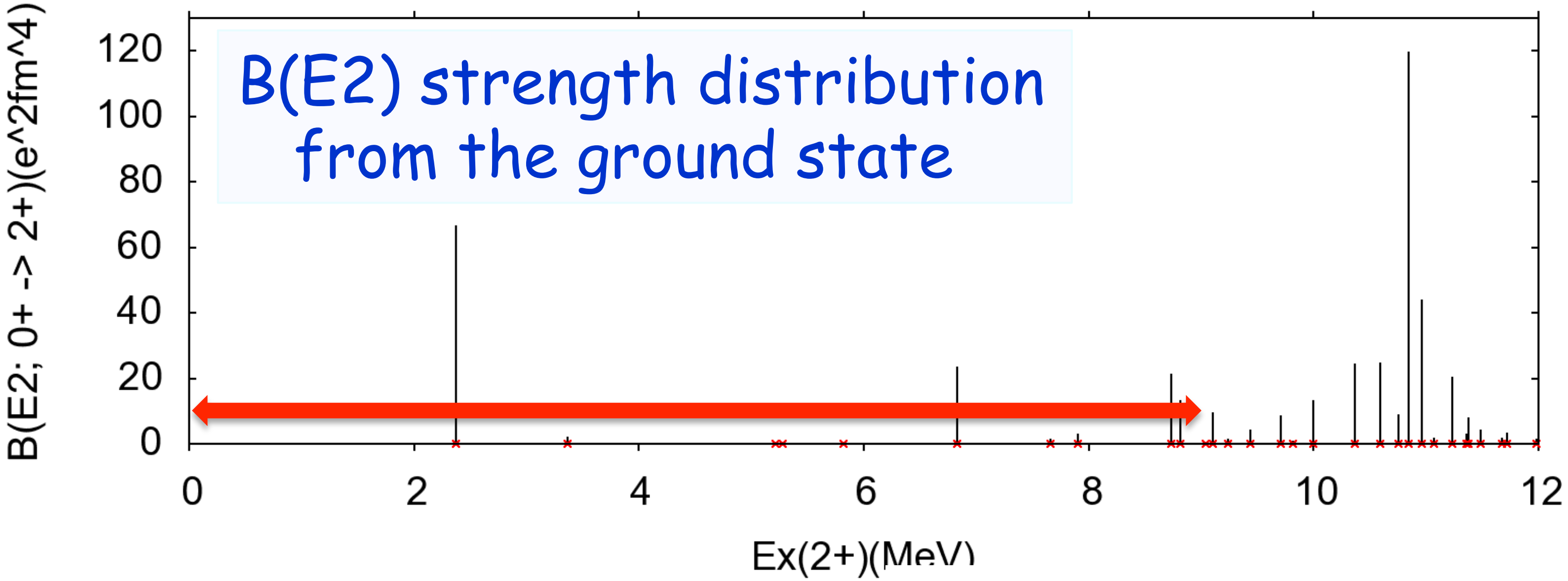
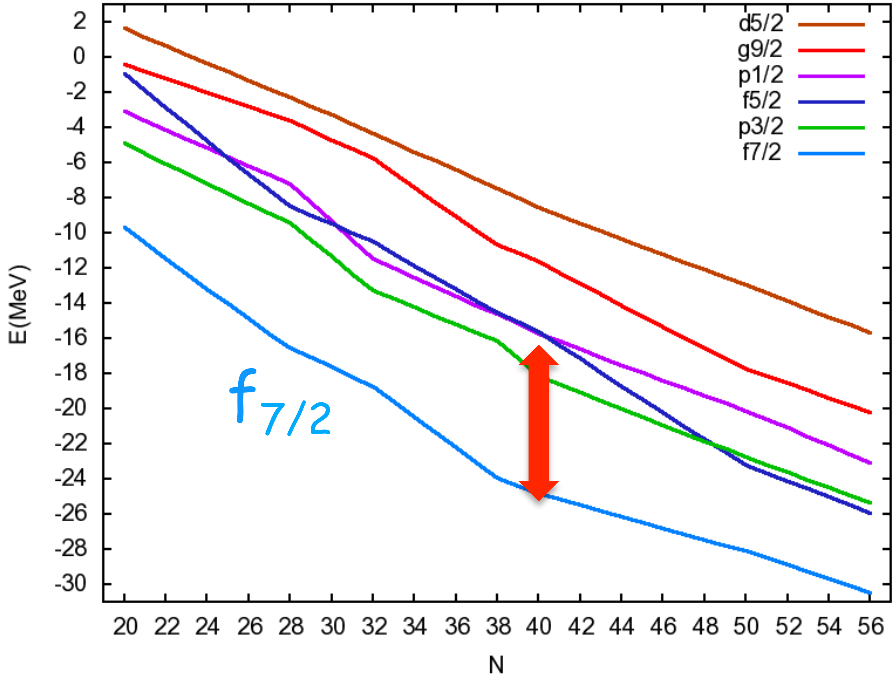


Figure 12. $E(4_1^+) - E(2_1^+)$ systematics for the $28 < Z, N < 50$ region (similar to figure 3 from [29]).

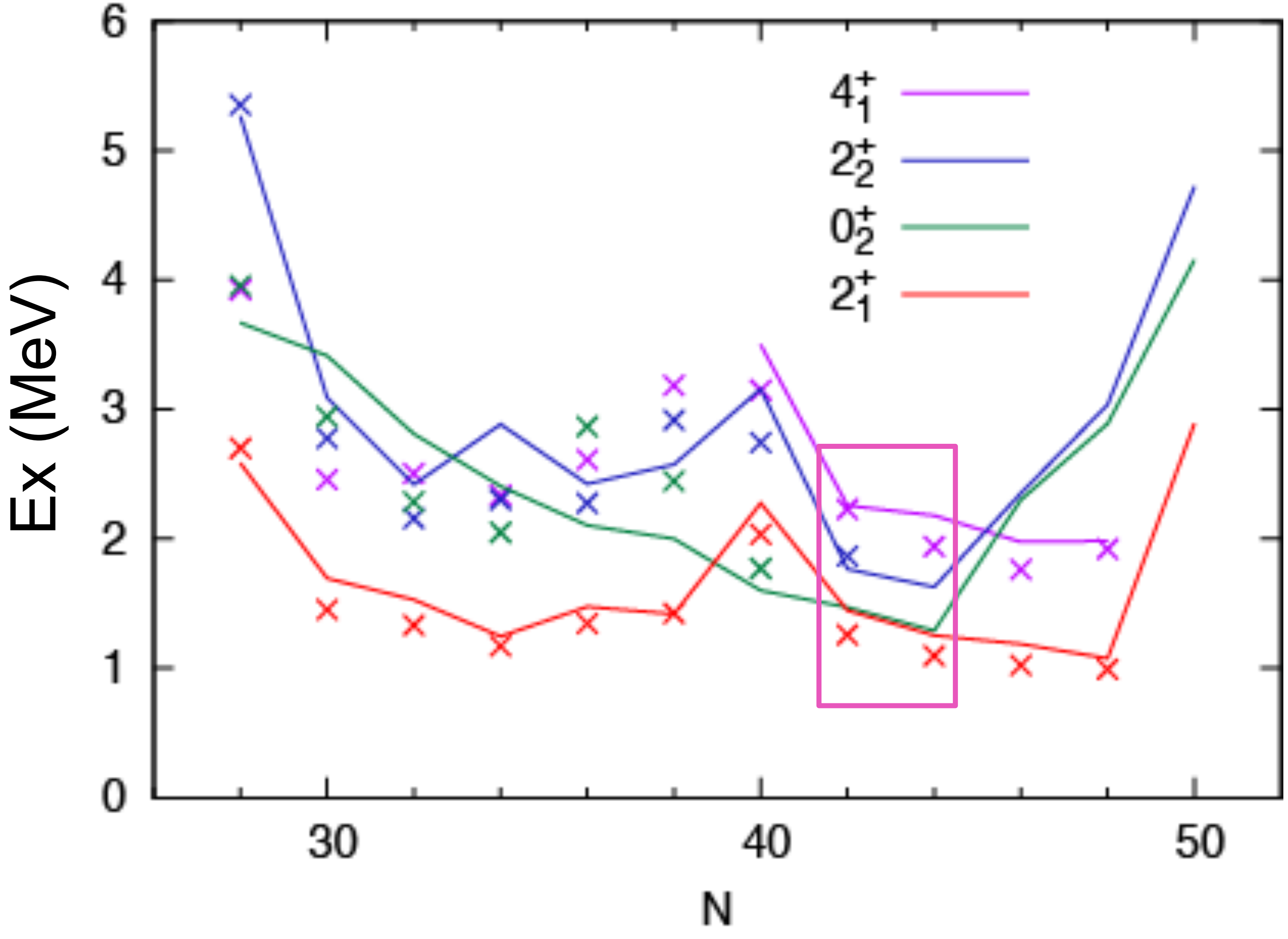
Where is the 2+ state built on the ground state of ^{68}Ni ?

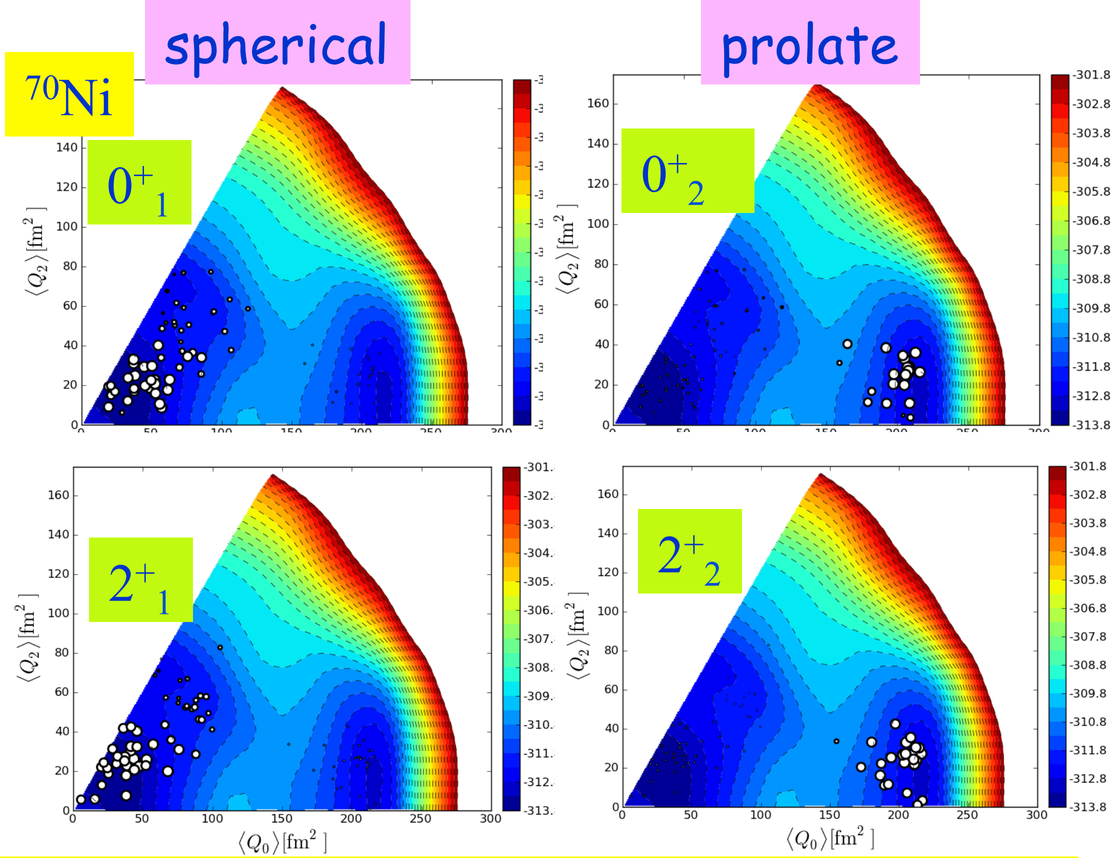

B(E2) strength distribution from the ground state



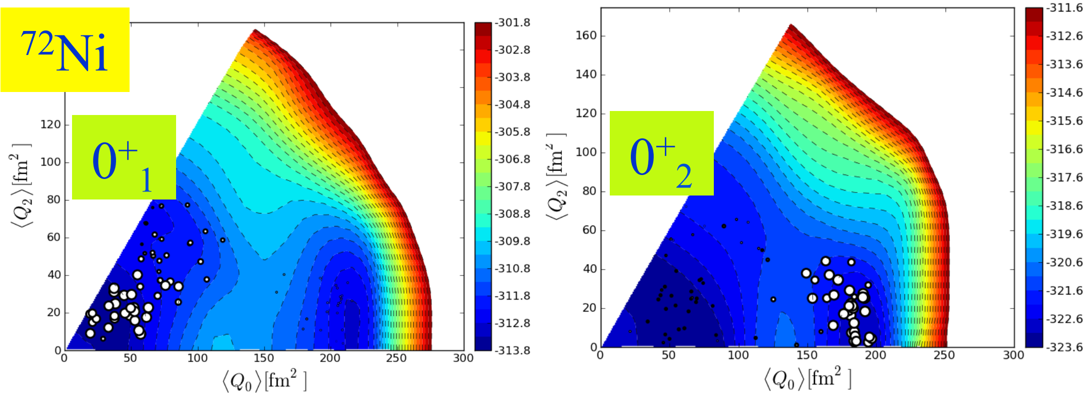
Proton single-particle energies for Z=28

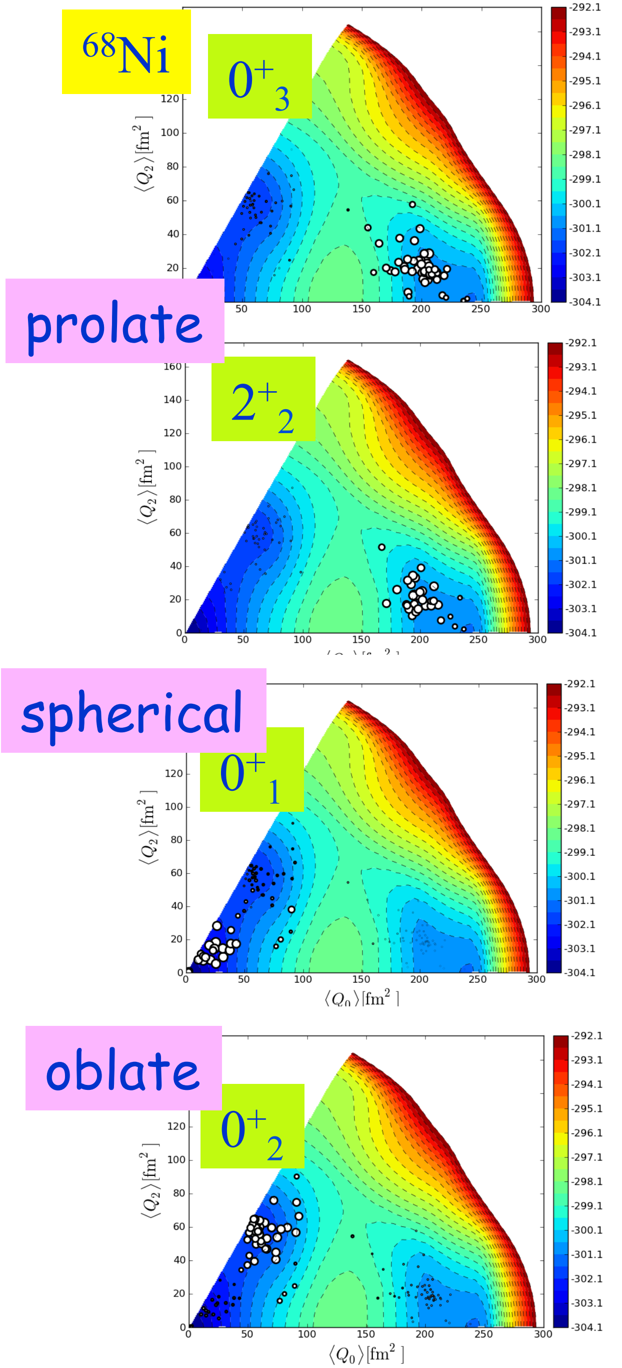
Excitation energies of Ni isotopes



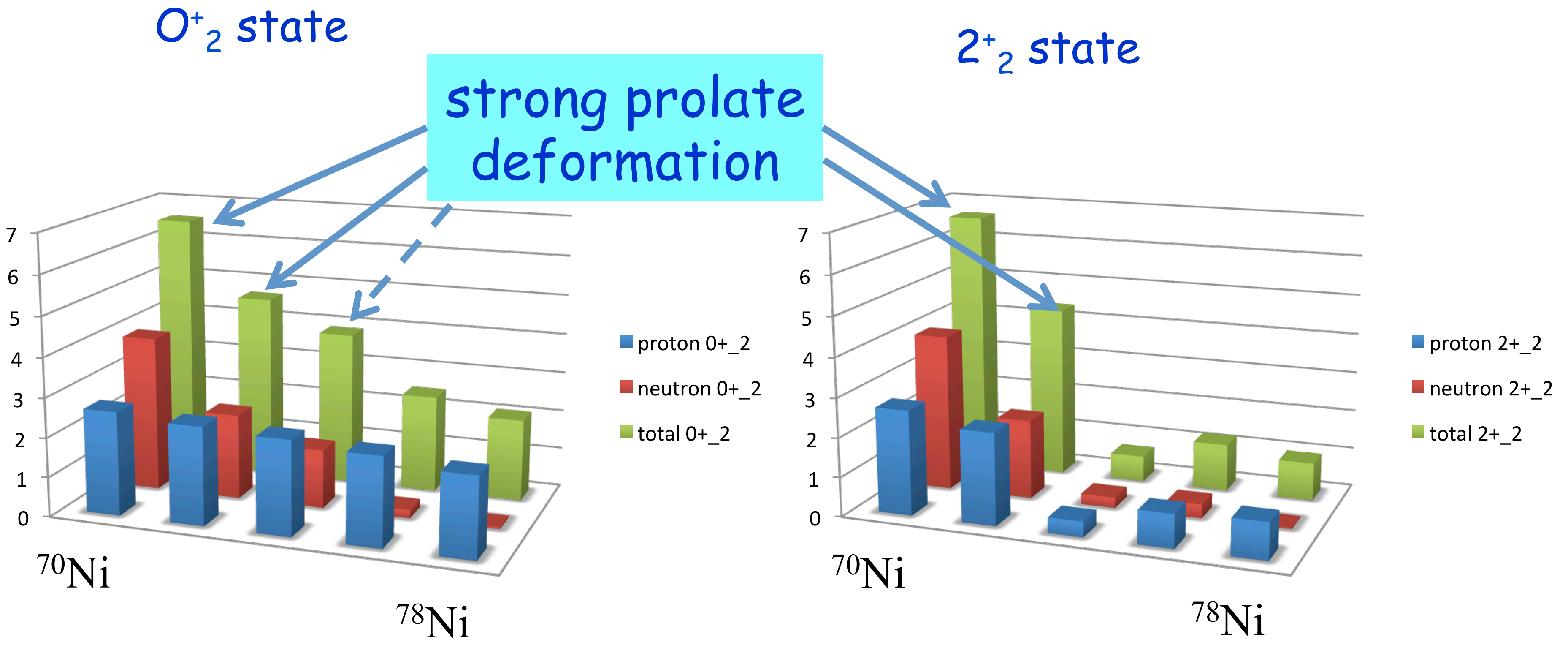


spherical and prolate still coexist !





Number of protons and neutrons excited across Z=28 or N=40 magic numbers

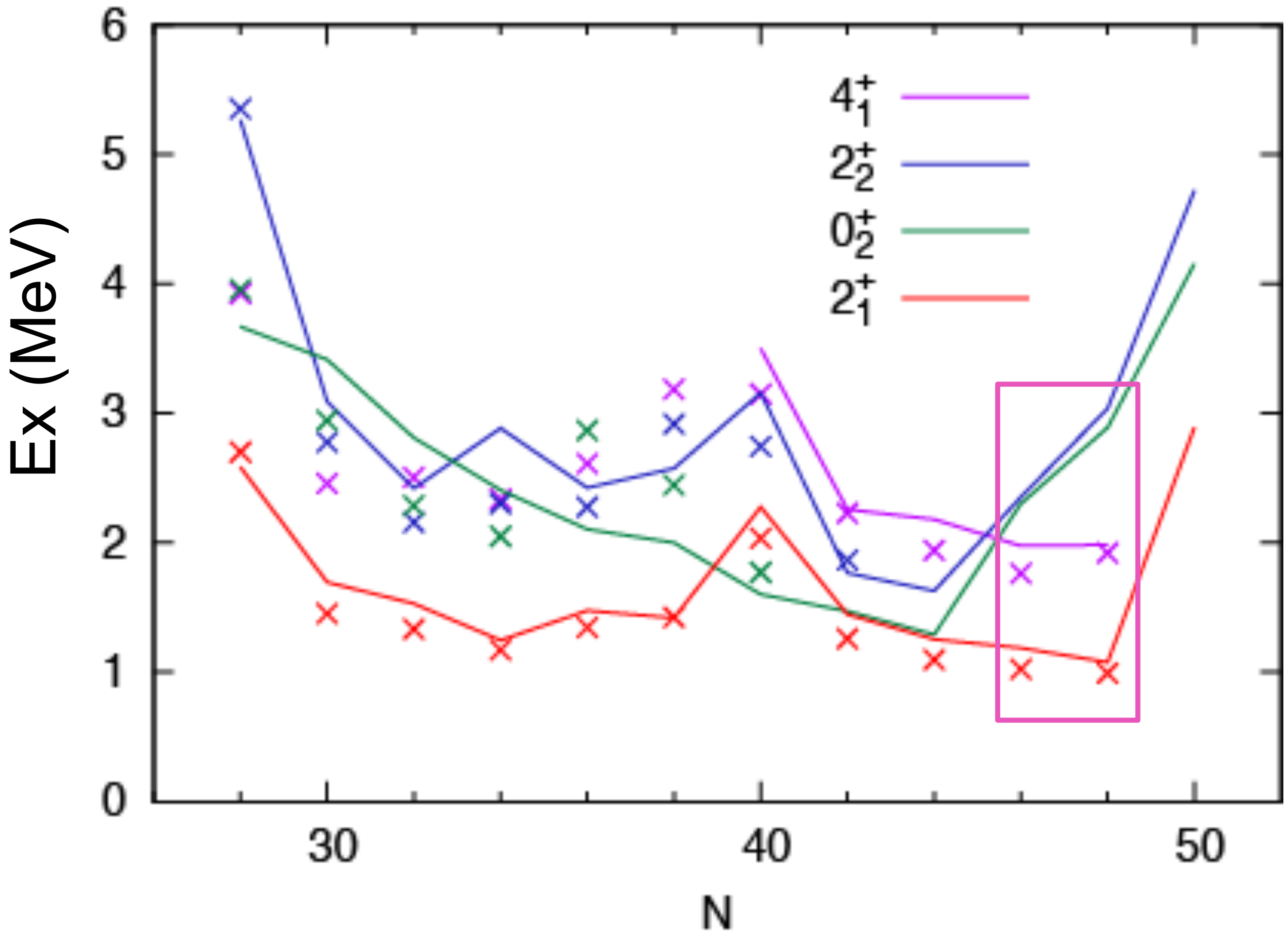


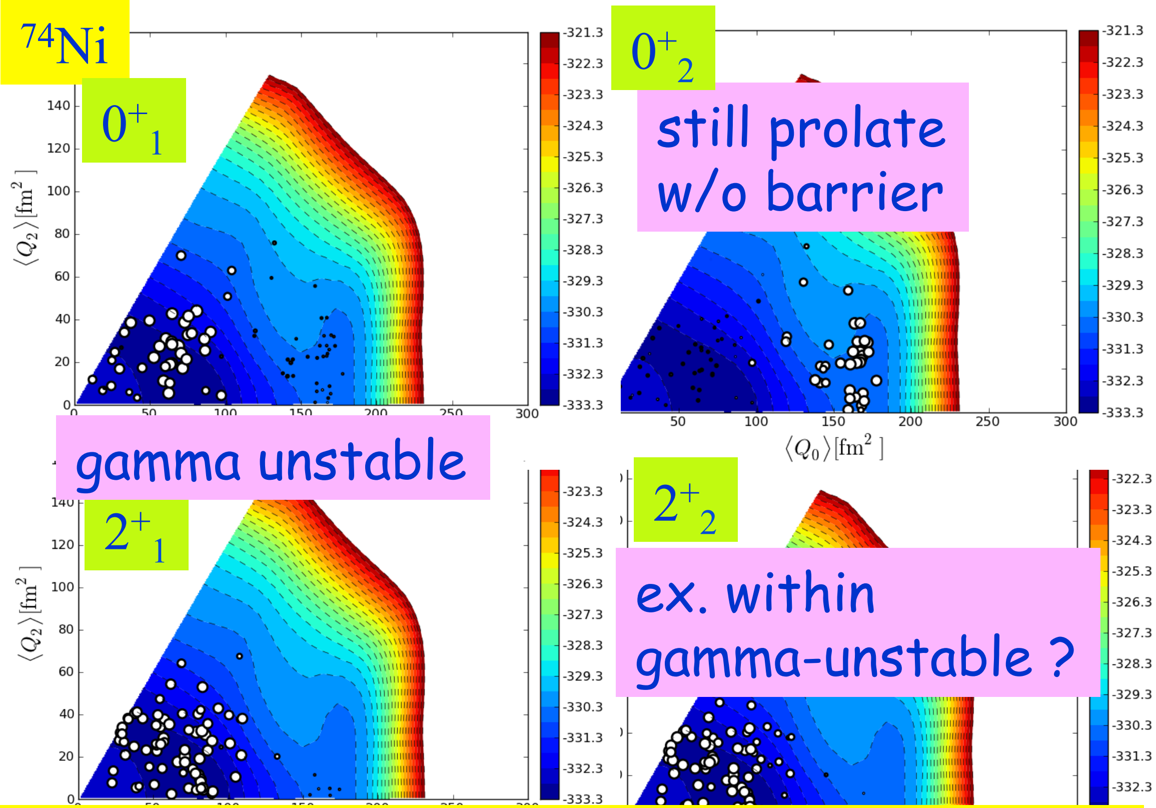
0^+_2 state

2^+_2 state

strong prolate deformation

Excitation energies of Ni isotopes





^{74}Ni

0^+_1

gamma unstable

2^+_1

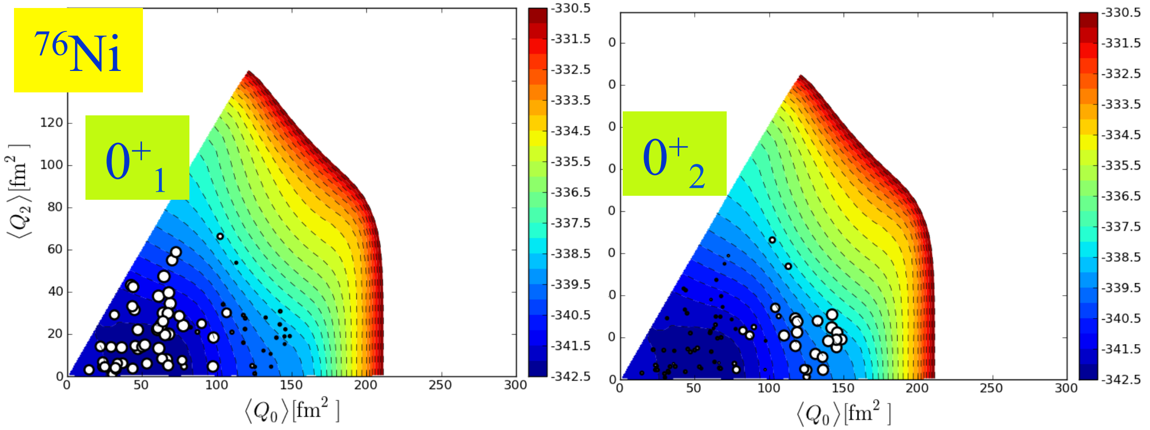
0^+_2

still prolate w/o barrier

2^+_2

ex. within gamma-unstable ?

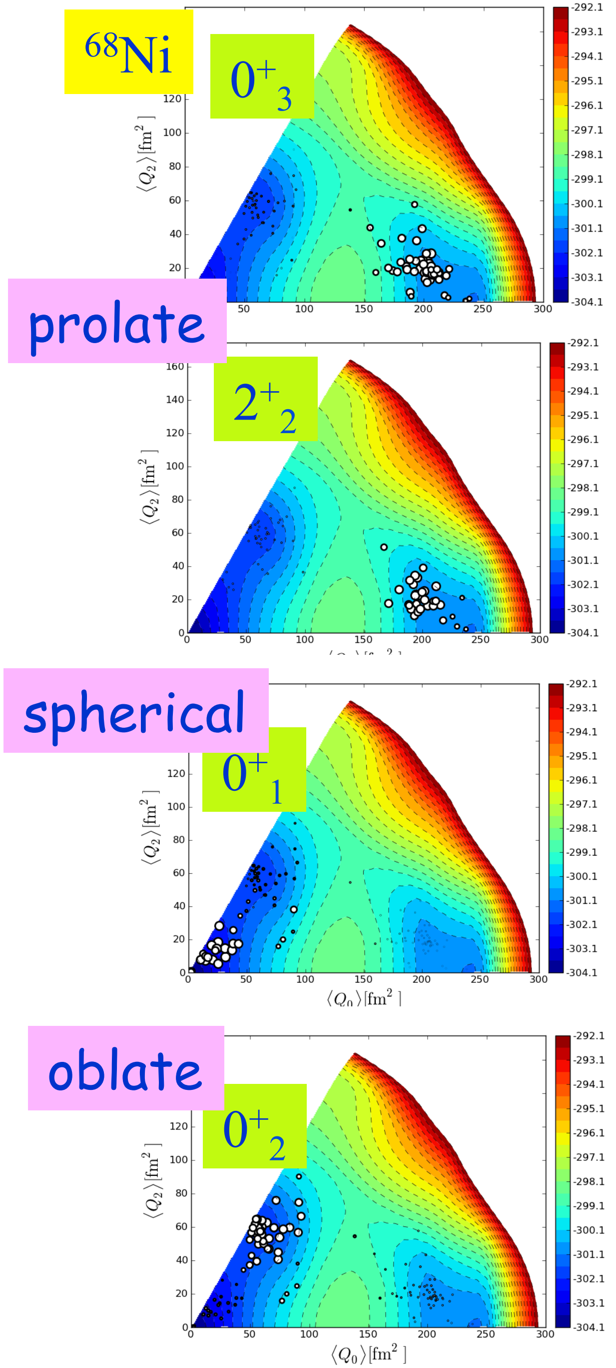
γ-unstable and prolate but separated



^{76}Ni

0^+_1

0^+_2



^{68}Ni

0^+_3

prolate

2^+_2

spherical

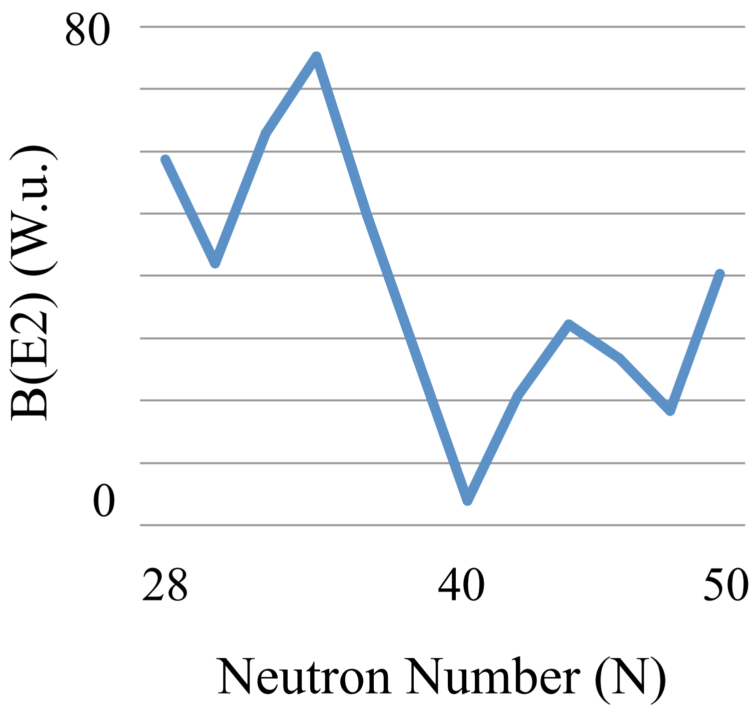
0^+_1

oblate

0^+_2

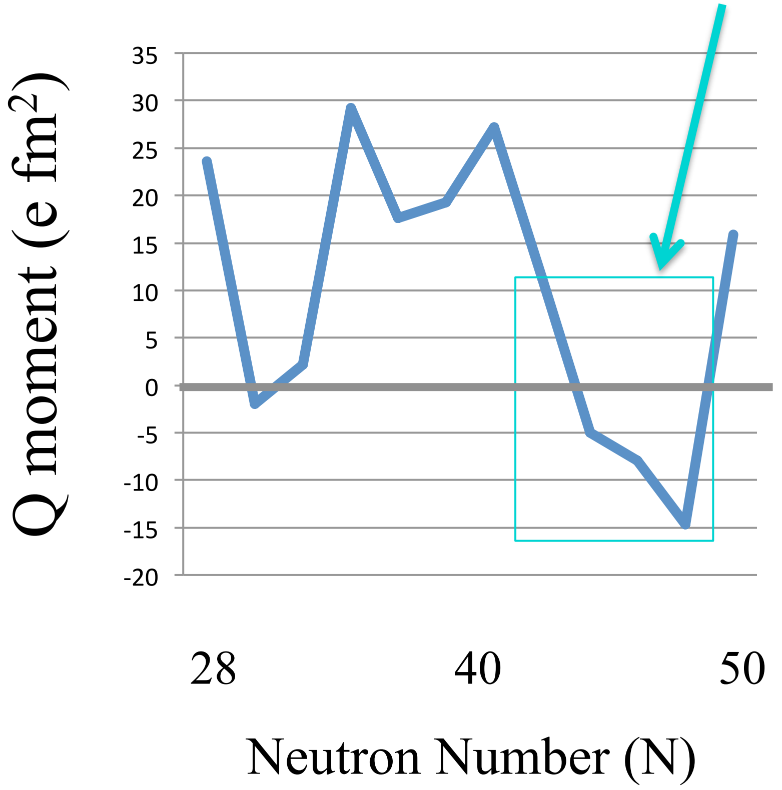
$B(E2;\ 0^+_1 \rightarrow 2^+_1)$

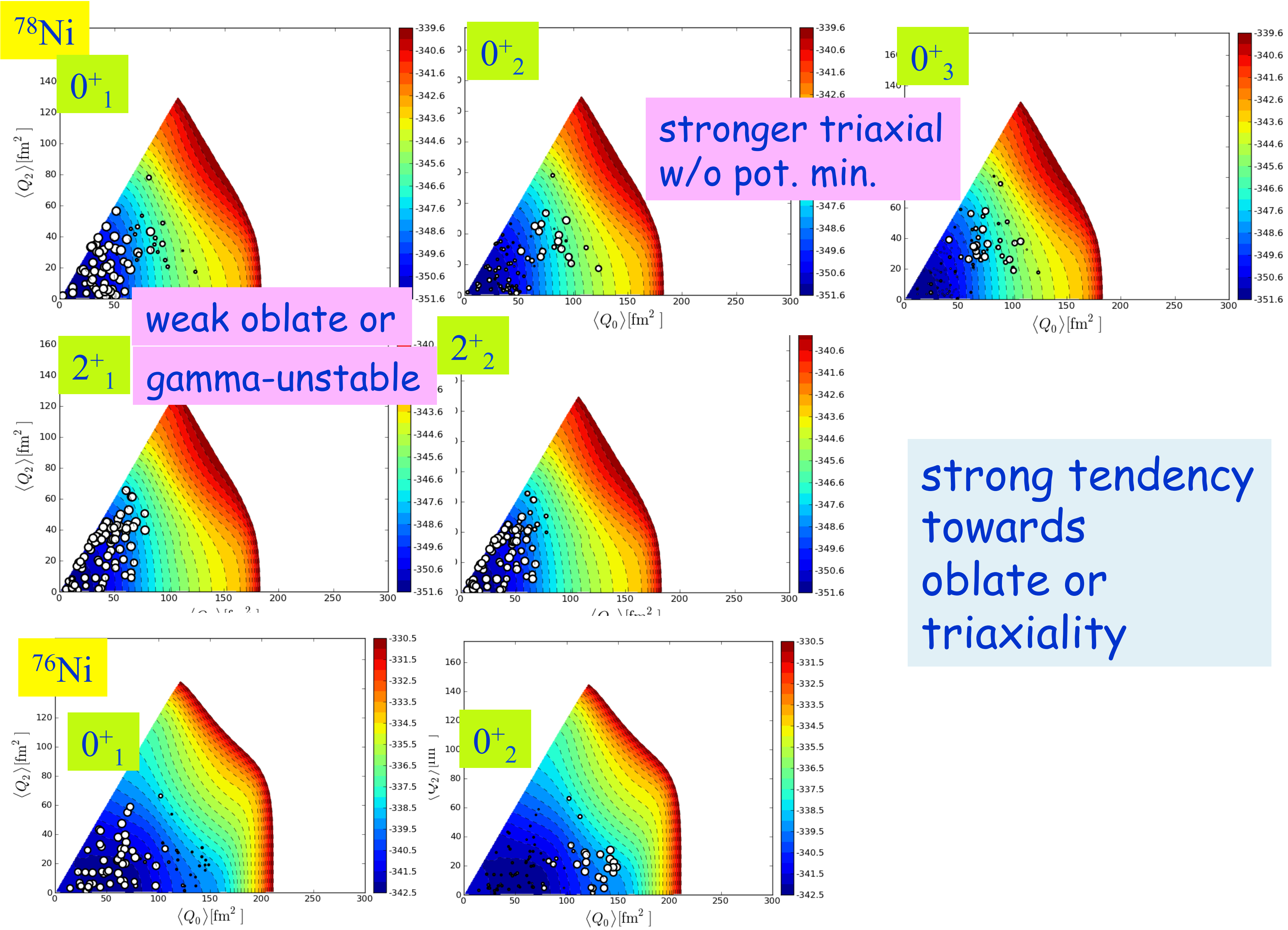
modestly large



Quadrupole moment (2^+_1)

small magnitude
(~seniority ?)

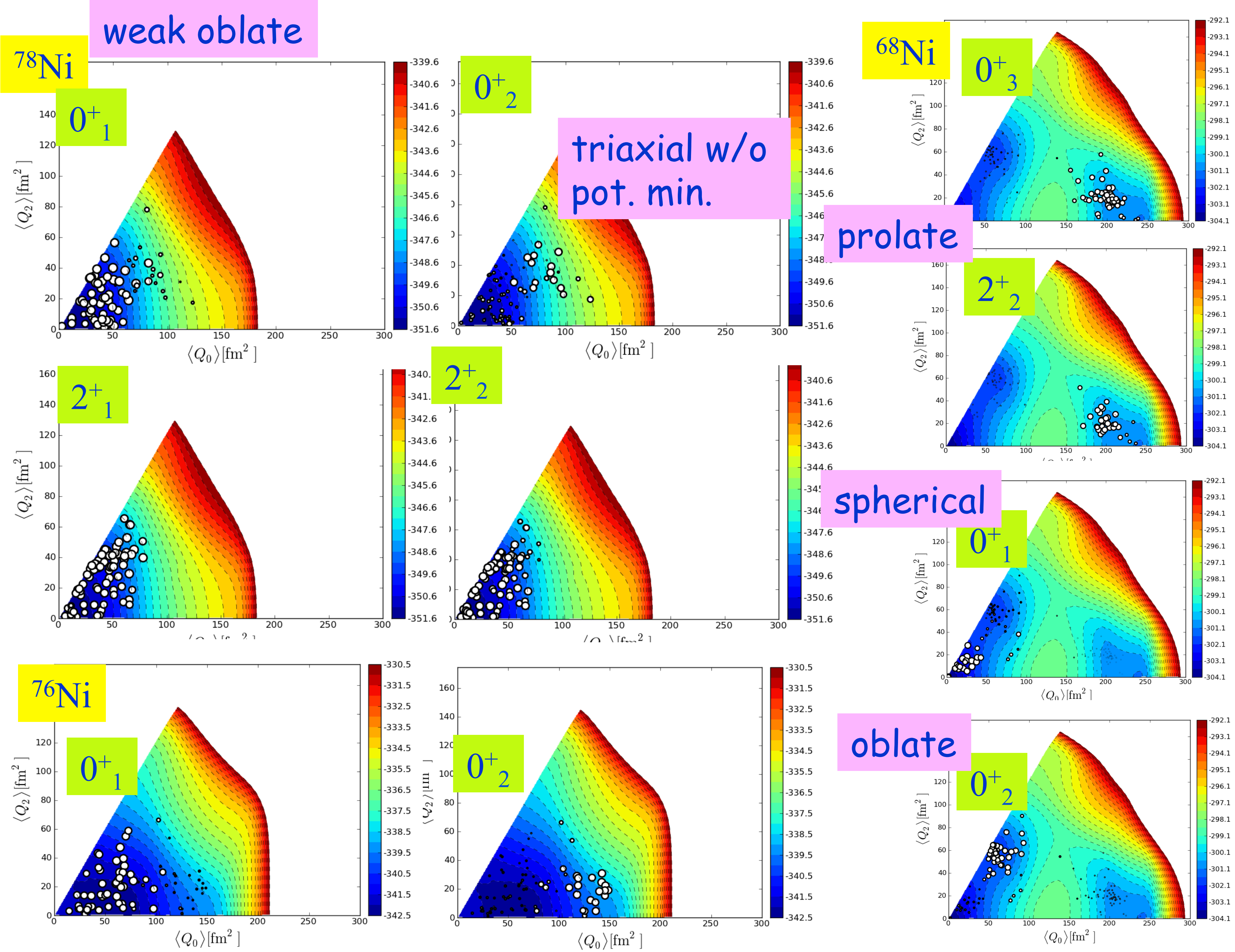




stronger triaxial w/o pot. min.

weak oblate or gamma-unstable

strong tendency towards oblate or triaxiality



weak oblate

^{78}Ni

0^+_1

0^+_2

triaxial w/o pot. min.

2^+_1

2^+_2

^{76}Ni

0^+_1

0^+_2

^{68}Ni

0^+_3

prolate

2^+_2

spherical

0^+_1

oblate

0^+_2

Summary

1. Novelties in effects of nuclear forces on the structure of exotic nuclei (e.g. evolution of shells, **shapes**, …)

2. Shapes can be studied well by Advanced Monte Carlo Shell model
   - quantum Monte Carlo + variational + variance-based extrapolation
   - "*intrinsic shapes*" of basis vectors (even for 0^+)

3. Exotic Ni isotopes
   - coexistence of three phases (spherical, oblate, prolate) in ^{68}Ni
     within 3 MeV all appear with beta ~ 0, -0.2, +0.4
     not simple particle-hole excitations, contrary to some anticipations
   - their evolutions with increasing *N*
     low-lying prolate in ^{70,72}Ni, while γ-unstable shape in ^{74,76}Ni

4. One shape (per one nucleus) -> Multi-shape paradigm for exotic nuclei

Different "shape phases" coexist partly due to shell structure
(ex. reduced and/or configuration dependent gaps)
-> instabilities, critical phenomena, … due to correlations
=> another new frontier where large-scale computation

Collaborators

Y. Tsunoda	Tokyo	Ni isotopes

Y. Utsuno	JAEA
N. Shimizu	Tokyo
M. Honma	Aizu
T. Mizusaki	Senshu U.
T. Abe	Tokyo
B.A. Brown	MSU

Shimizu

Abe

T. Suzuki	Nihon U.
N. Tsunoda	(Tokyo)
K. Tsukiyama	(Tokyo)
M. H.-Jensen	Oslo/MSU
Y. Akaishi	RIKEN

A. Schwenk	Darmstadt
J. Holt	Darmstadt

END

Major computational work in MCSM :
Projection of deformed Slater determinants
(many-body basis vectors) onto good J and parity

Rotation with three Euler angles numerically
-> about 50,000 mesh points of the angles

K computer (in Kobe)
10 peta flops machine
(3rd fastest)

HPCI Strategic Programs for Innovative Research (SPIRE)
Field 5 "The origin of matter and the universe"

One of 4 groups is for nuclear structure (mainly MCSM)

Example : 8^+ ^{68}Ni 7680 cpu core x 14 h

ARIS2014 Advances in Radioactive Isotope Science) *

- 2nd of the ARIS series, Sister of EMIS -

Flagship conference on exotic nuclei / radioactive ion beams

Former ENAM + RNB (in its science part)

2-6 June 2014

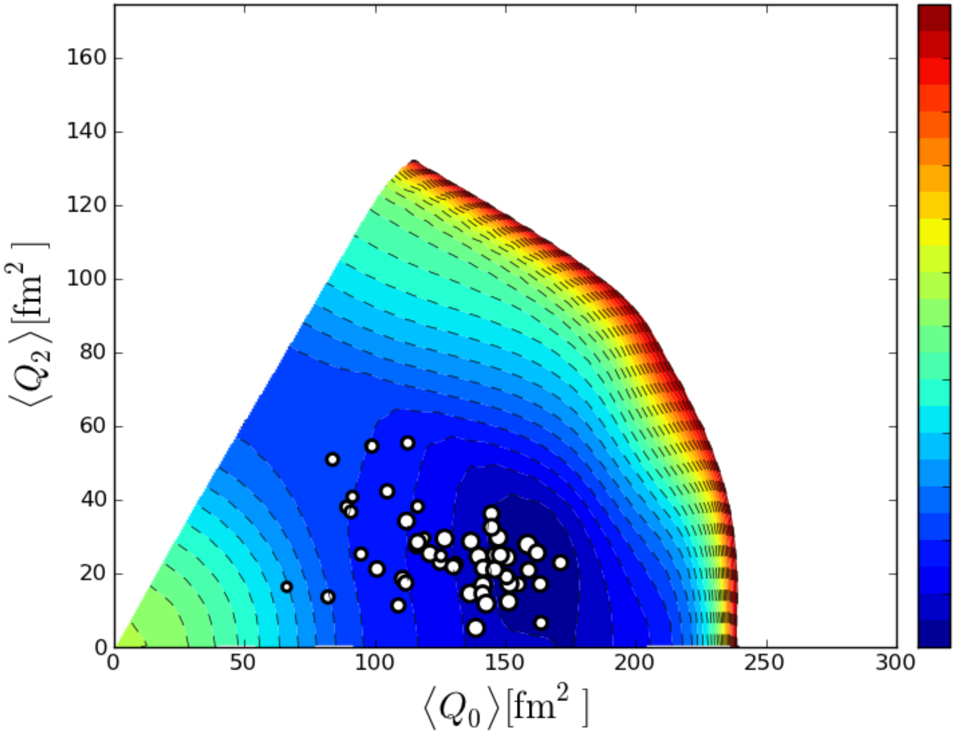
ITO International Research Center (in the campus of University of Tokyo)
伊藤国際学術研究センター (東大本郷キャンパス、赤門脇）
Public lectures on 1 June

Hosts: RIKEN Nishina Center
The University of Tokyo (CNS)

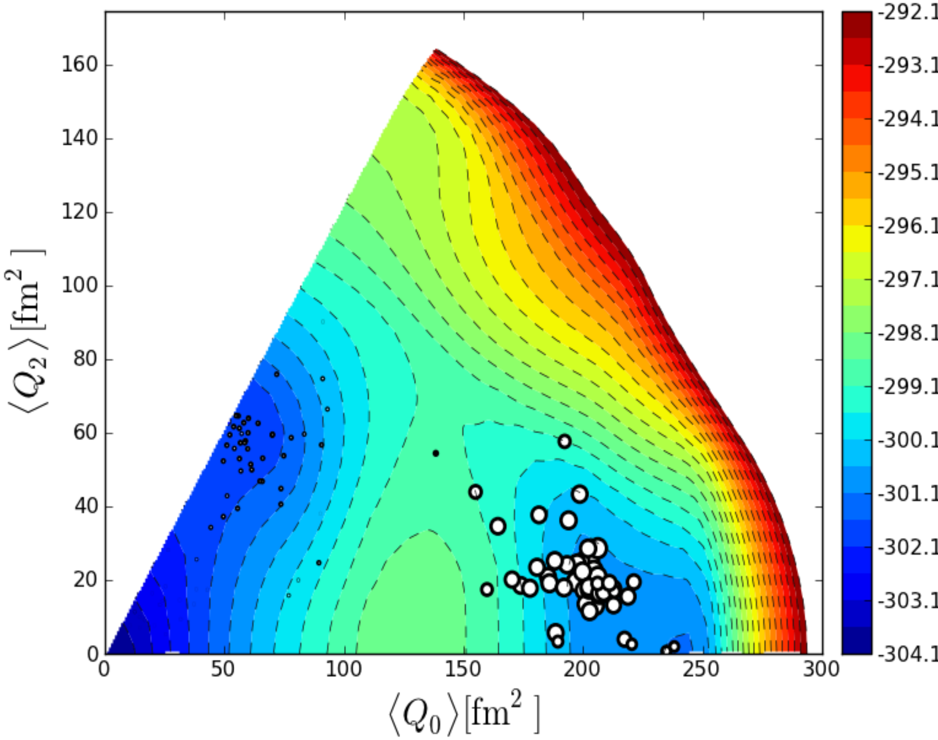
Chair : H. Enyo
Co-chair : T. Otsuka
Secretary : T. Motobayashi

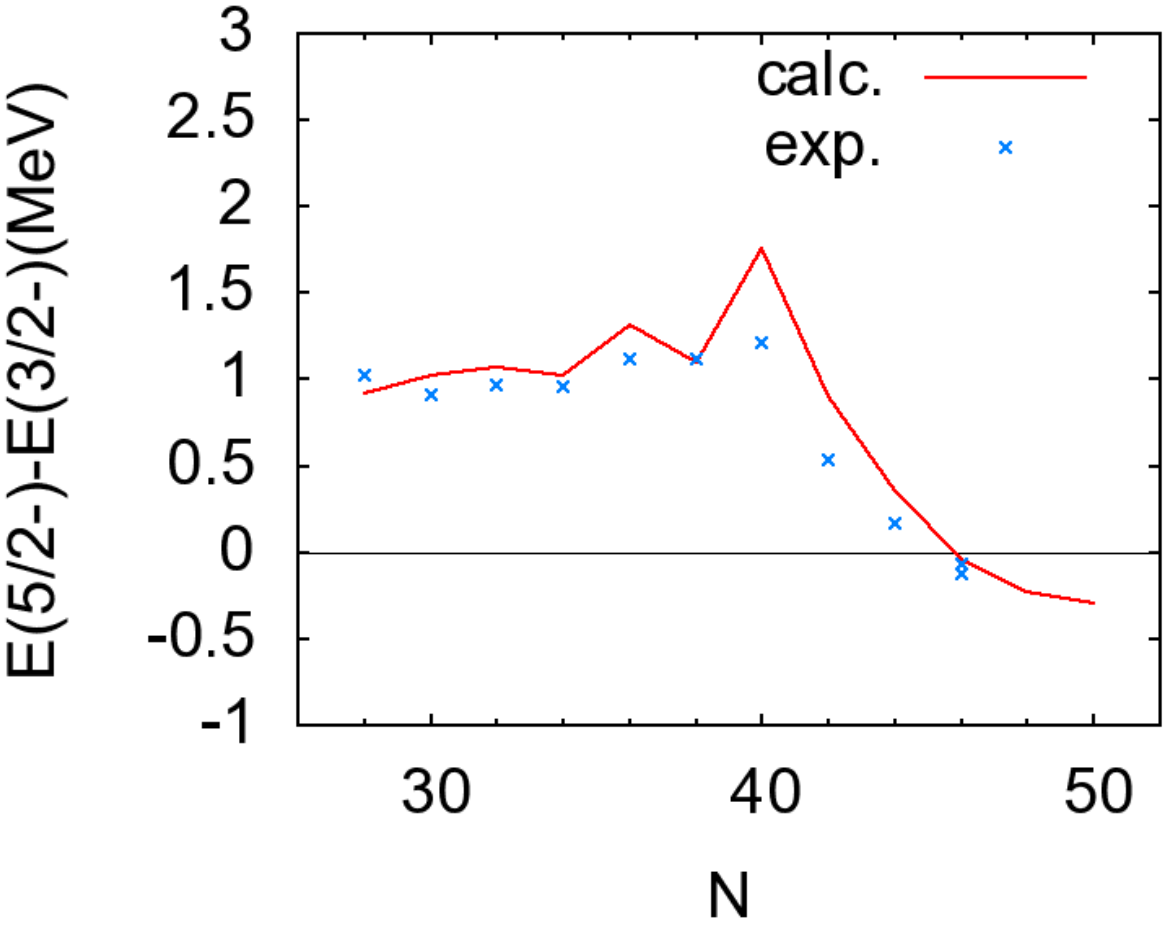
Web page in preparation.

^{64}Cr 0^+_1



^{68}Ni 0^+_3

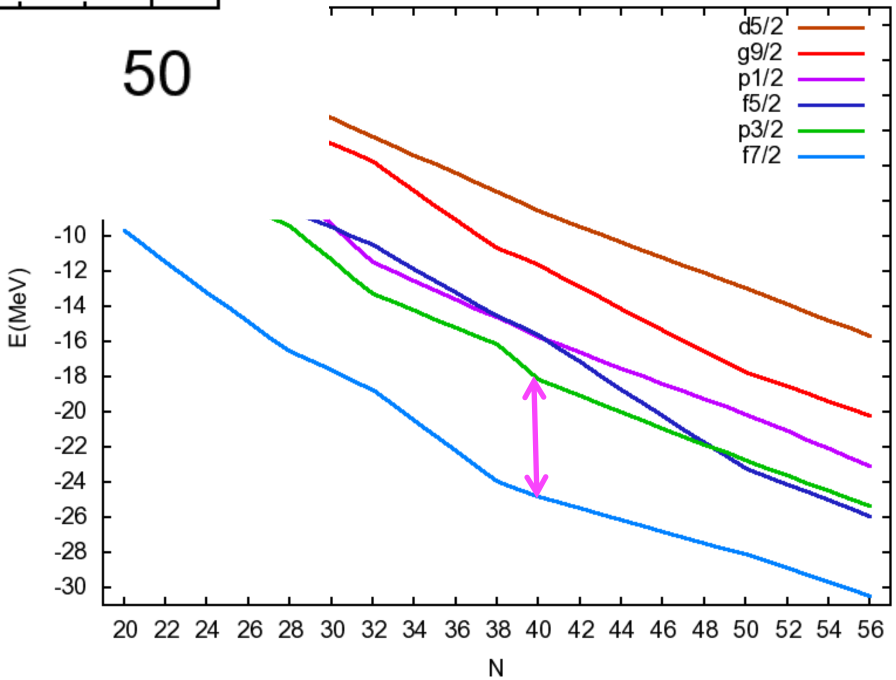




$5/2^-$ of Cu isotopes relative to $3/2^-$

Flanagan et al.
PRL 103, 142501
(2009)

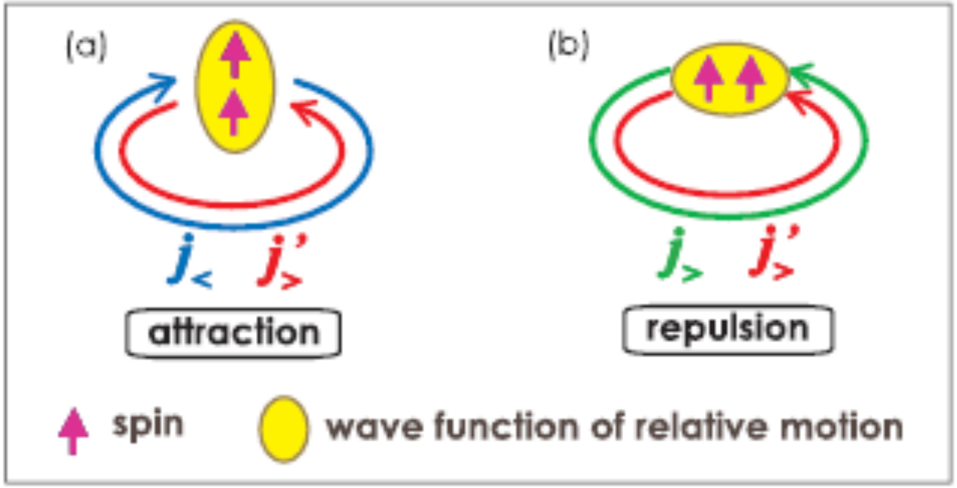
Proton single-particle energies for Z=28

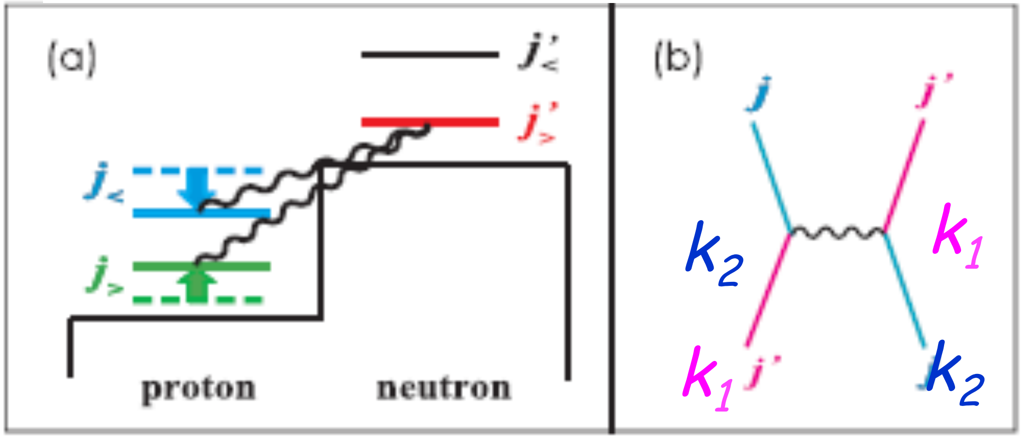


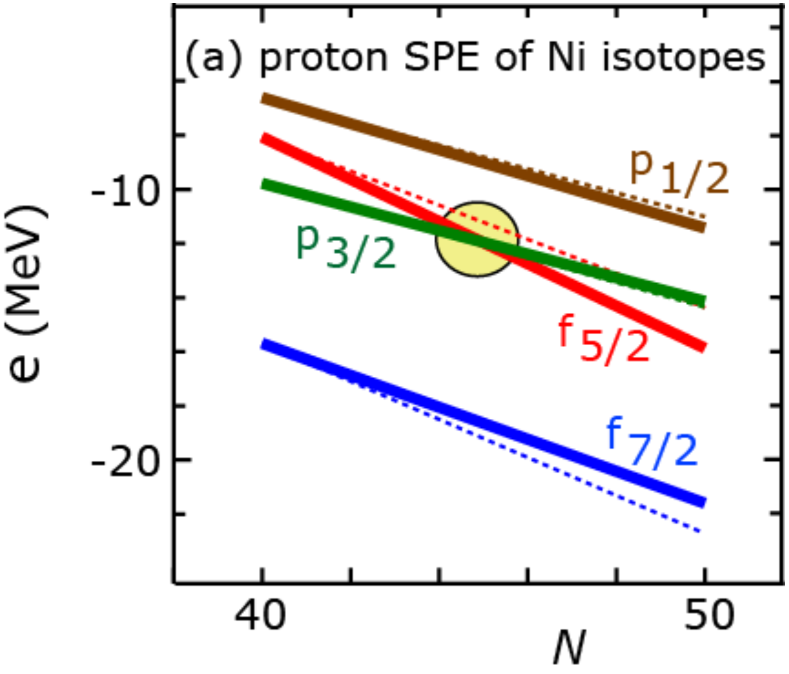
TO, Suzuki, et al.
PRL 95, 232502

Monopole component of tensor force

- An intuitive picture -

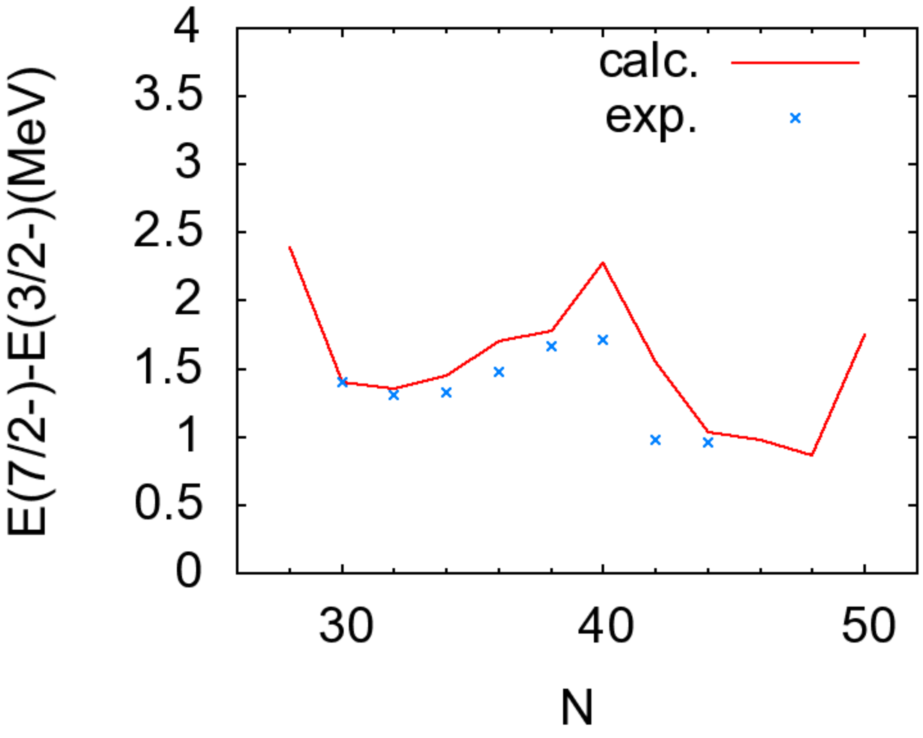






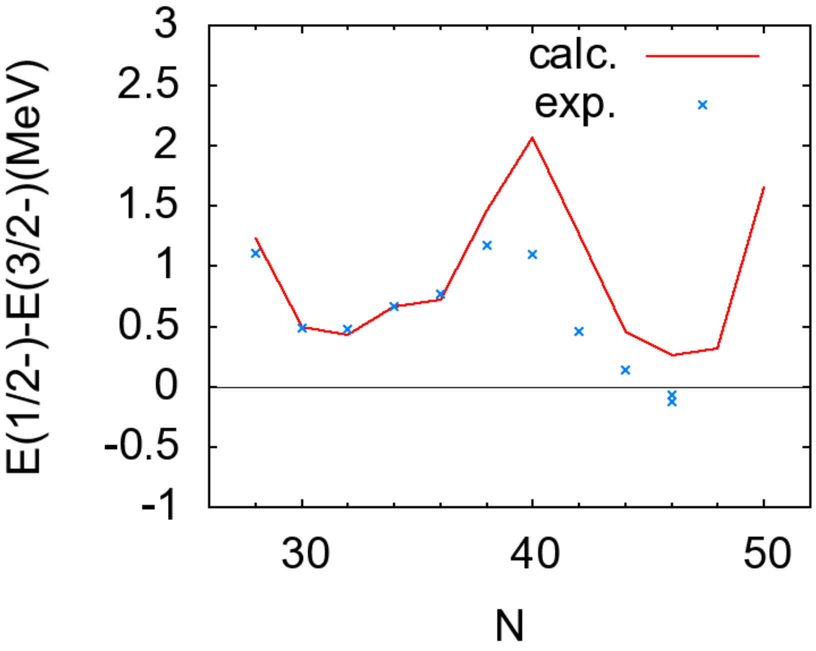
neutrons in $g_{9/2}$

Exp. nudat2



7/2⁻ of Cu isotopes relative to 3/2⁻

1/2⁻ of Cu isotopes relative to 3/2⁻



Outline

1. Introduction

2. Shape phase transitions in stable nuclei

3. Shape transitions in Si isotopes and tensor force

4. Advanced Monte Carlo Shell Model

5. Shape phase transitions in exotic Ni isotopes

6. Summary

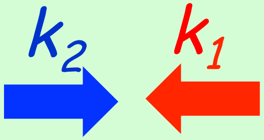
Monopole component of tensor force

- An intuitive picture -

TO, Suzuki, et al.
PRL 95, 232502

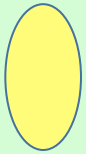
At collision point:

$$\Psi \propto e^{ik_1x_1}e^{ik_2x_2} + e^{ik_2x_1}e^{ik_1x_2} = 2\,e^{iKX}\cos(kx)$$



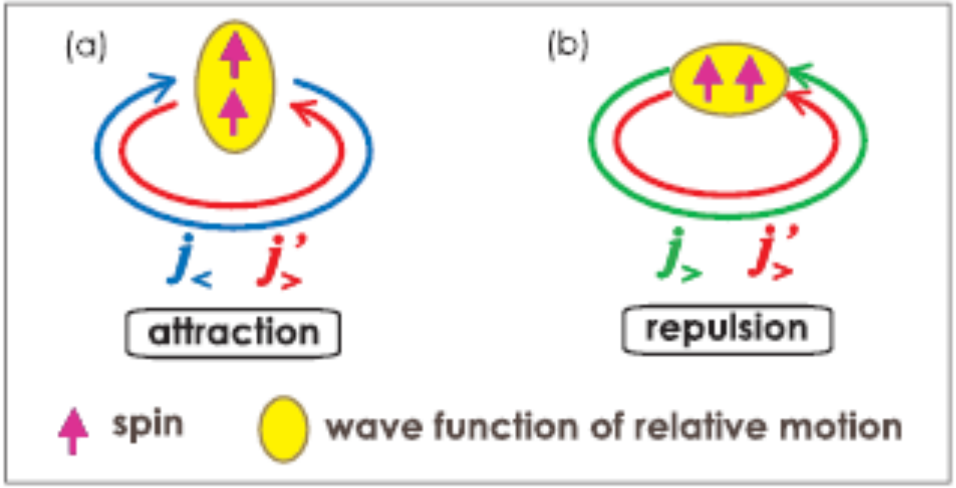
large relative momentum k

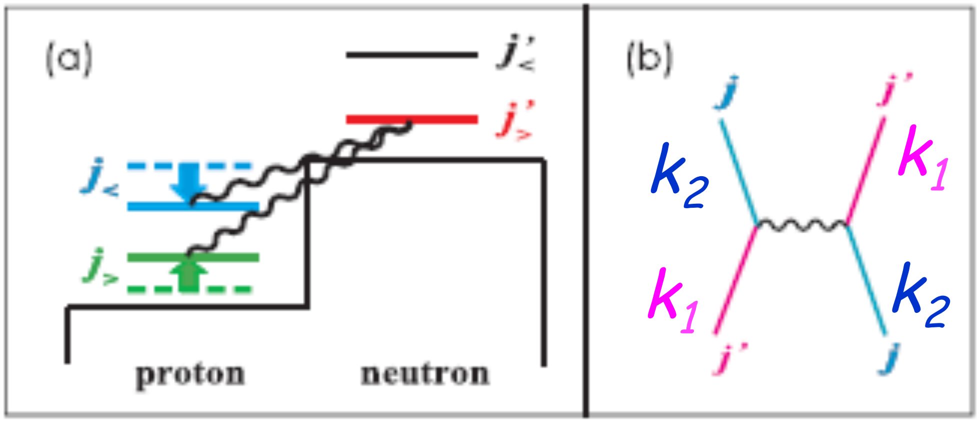
strong damping

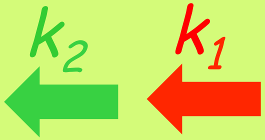


wave function of relative coordinate

$k = k_1 - k_2\,,\quad K = k_1 + k_2$

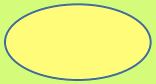






small relative momentum k

loose damping



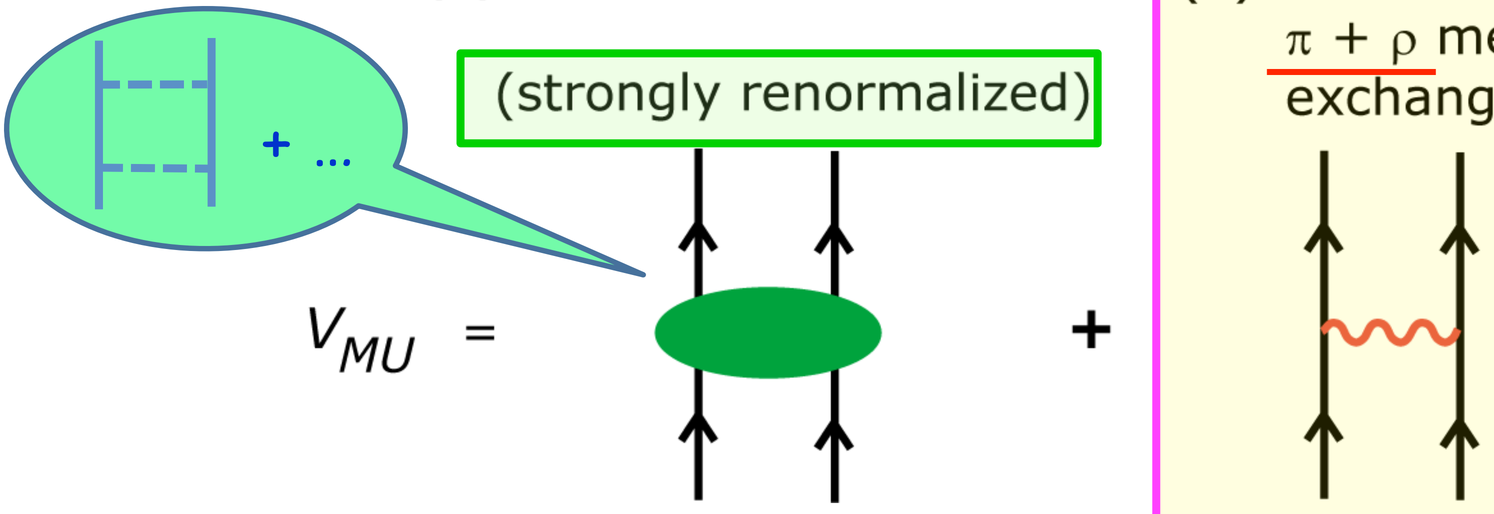
wave function of relative coordinate

Two major components in two-body nuclear force

(a) central force :

(strongly renormalized)

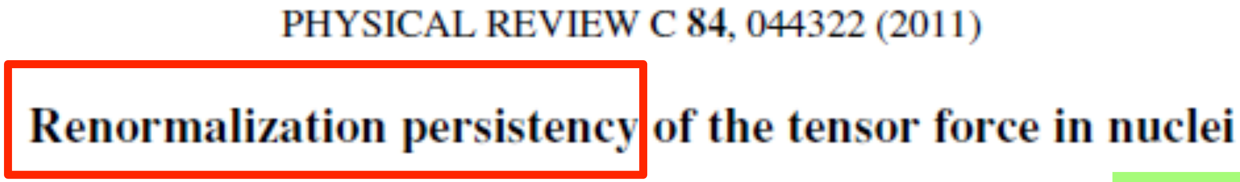
(b) tensor force :
$\pi + \rho$ meson exchange



in nuclear medium

almost equal

in free space



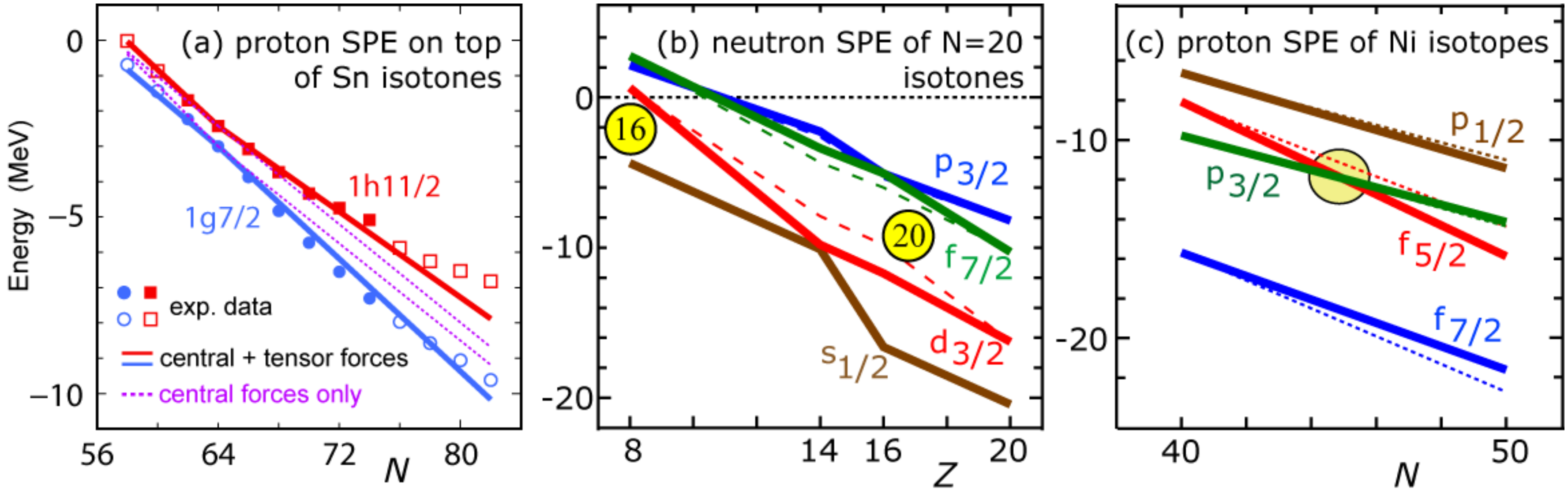
PHYSICAL REVIEW C 84, 044322 (2011)

Renormalization persistency of the tensor force in nuclei

N.Tsunoda, T.O., K.Tsukiyama, M.H.-Jensen

Shell evolution due to the tensor + central forces appears almost everywhere on the nuclear chart.

To appear in NuPECC News, Dec. 2012



Proton orbits on top of Sn core.

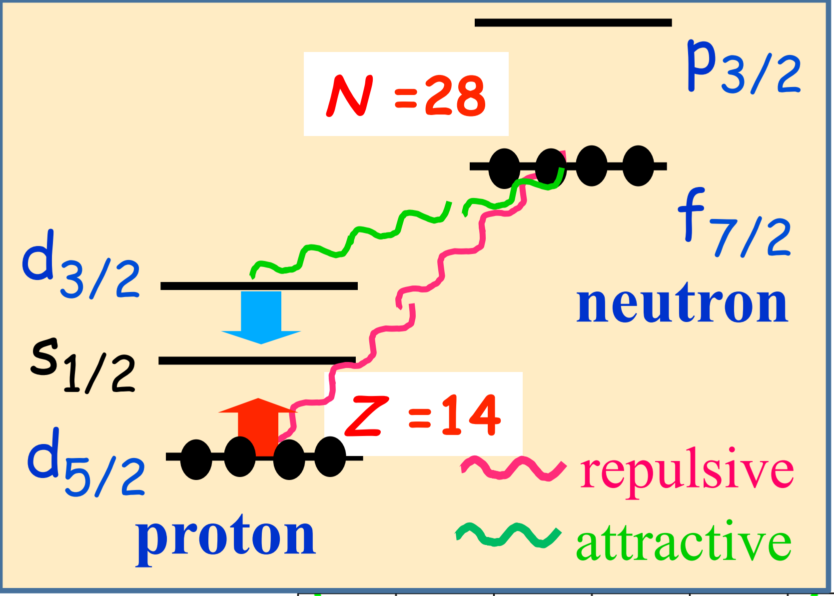
Emerging of magic number N=16, and disappearance of N=20.

Weakening of Z=28 gap and crossing between $f_{5/2}$ and $p_{3/2}$ -> exotic Ni isotopes

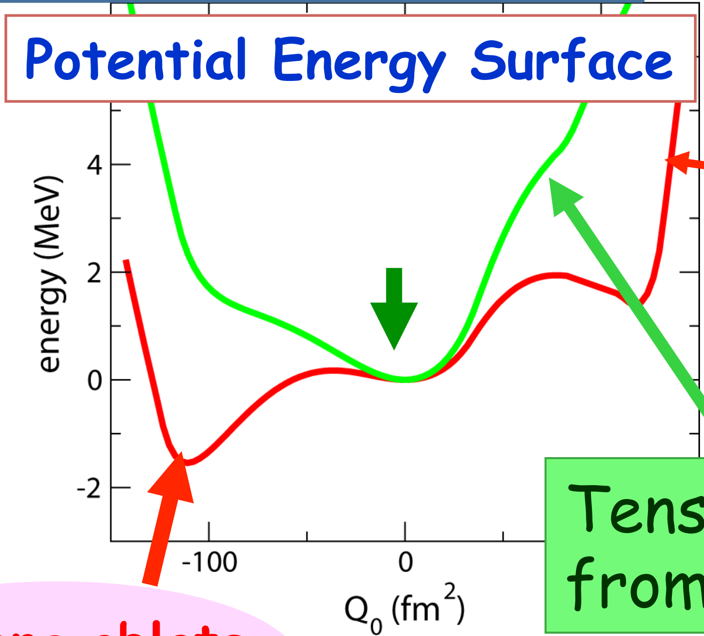
Otsuka, Suzuki and Utsuno, Nucl. Phys. A805, 127c (2008)

$^{42}_{14}\mathrm{Si}_{28}$

doubly magic ?

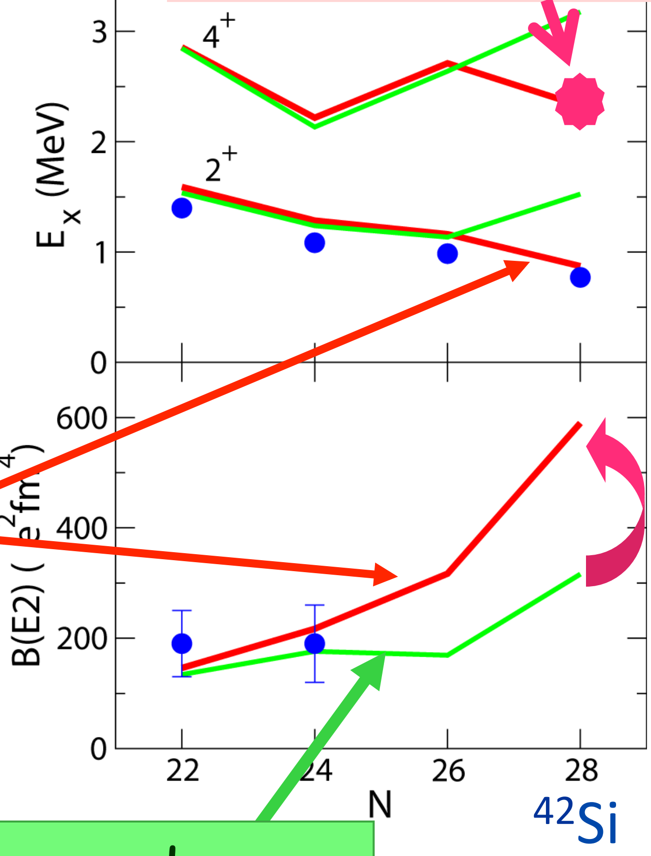


Potential Energy Surface



● exp.

(4+): RIBF data 2011



full

Tensor force removed from cross-shell interaction

Strong oblate Deformation

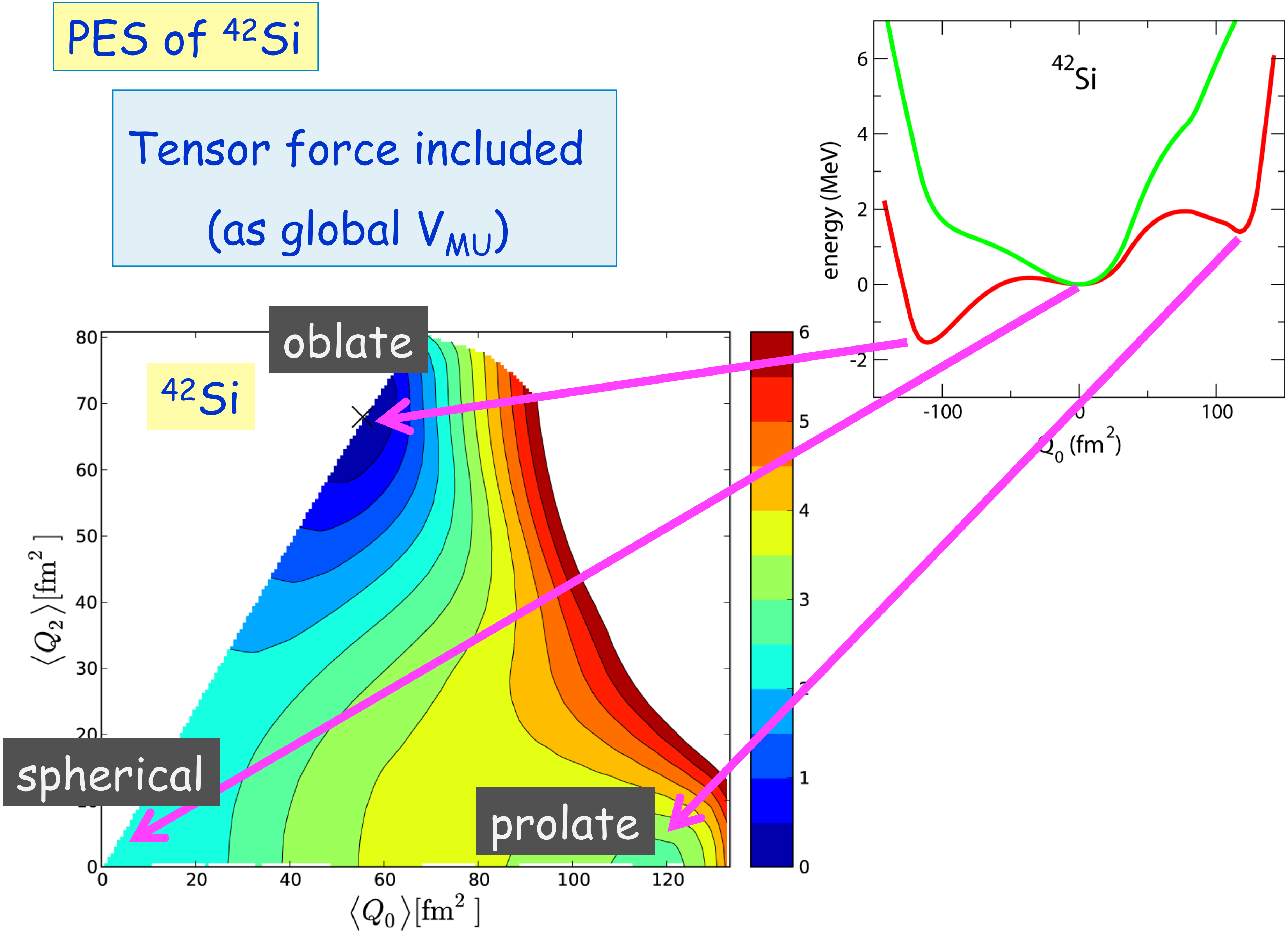
Other calculations (RMF, Gogny) show oblate shape.

^{42}Si 2+: *Bastin, Grévy et al., PRL 99 (2007) 022503*

PES of ^{42}Si

Tensor force included

(as global V_{MU})



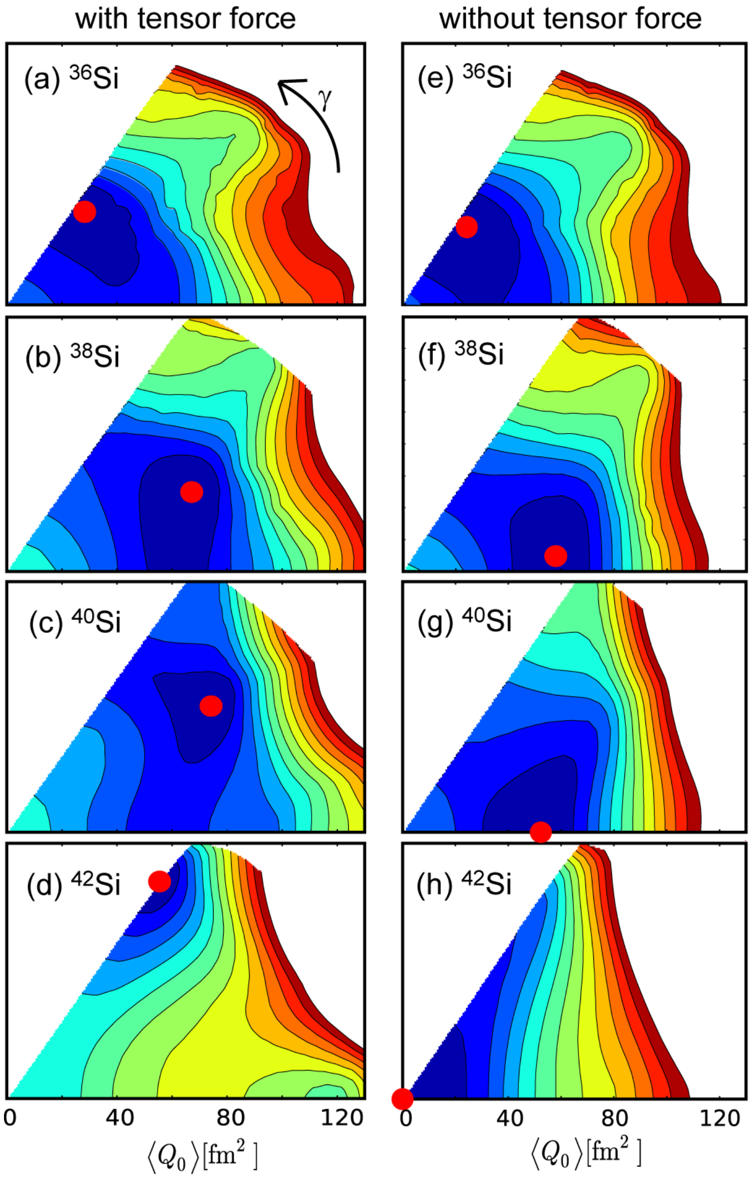
Exotic Si and S isotopes

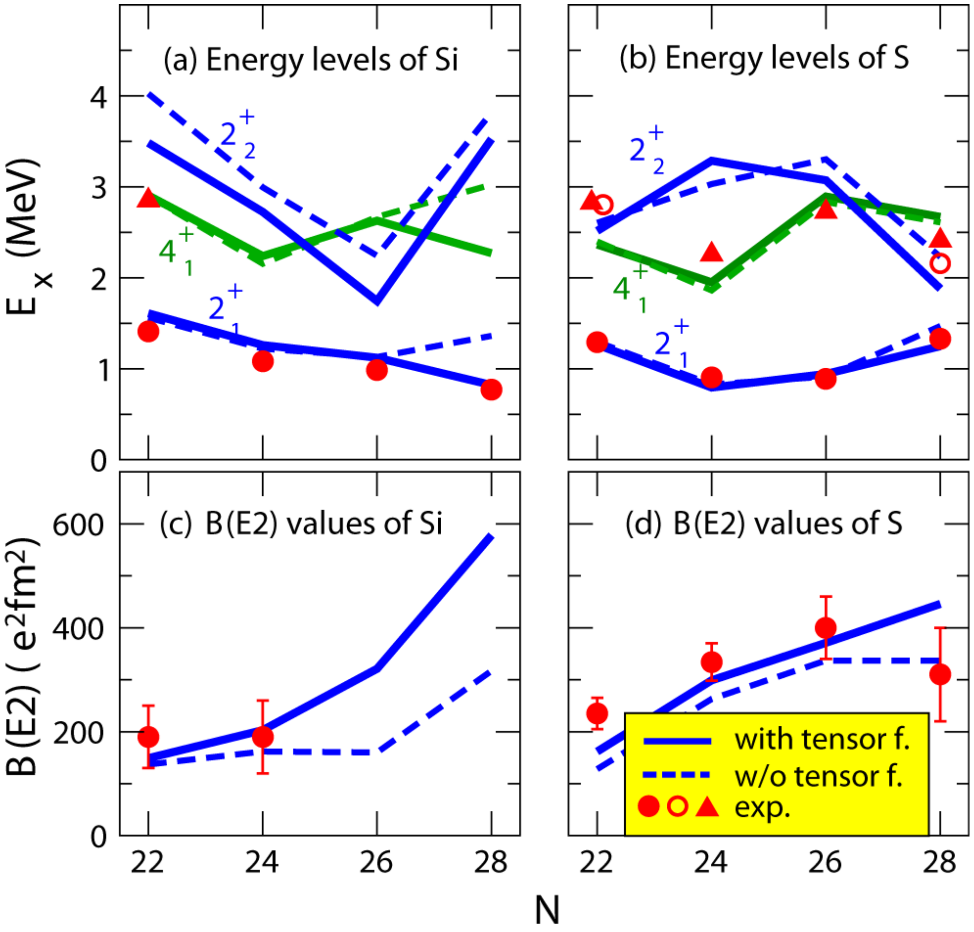
Utsuno, Otsuka, *et al.*, Phys. Rev. C (2012)

Shapes (PES)

Levels and B(E2)'s

Si



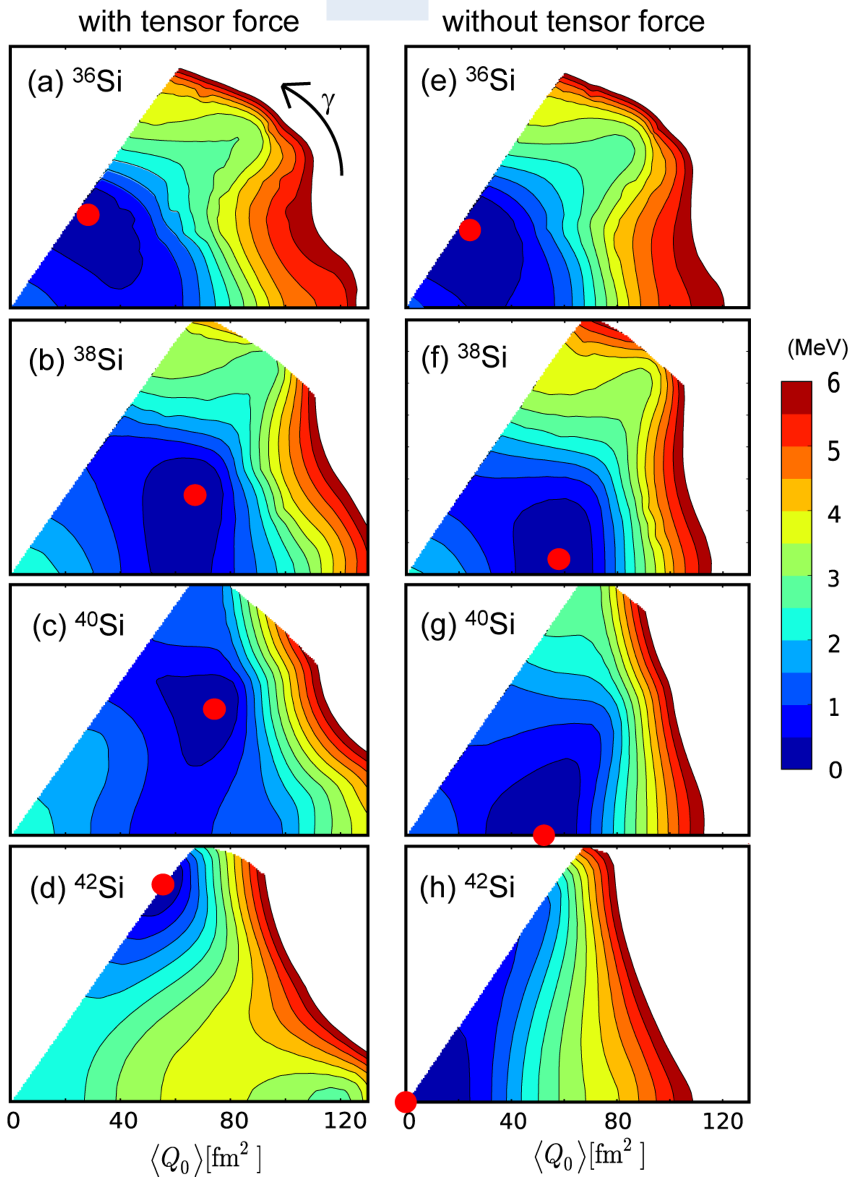


——— with cross shell (p-n) tensor force

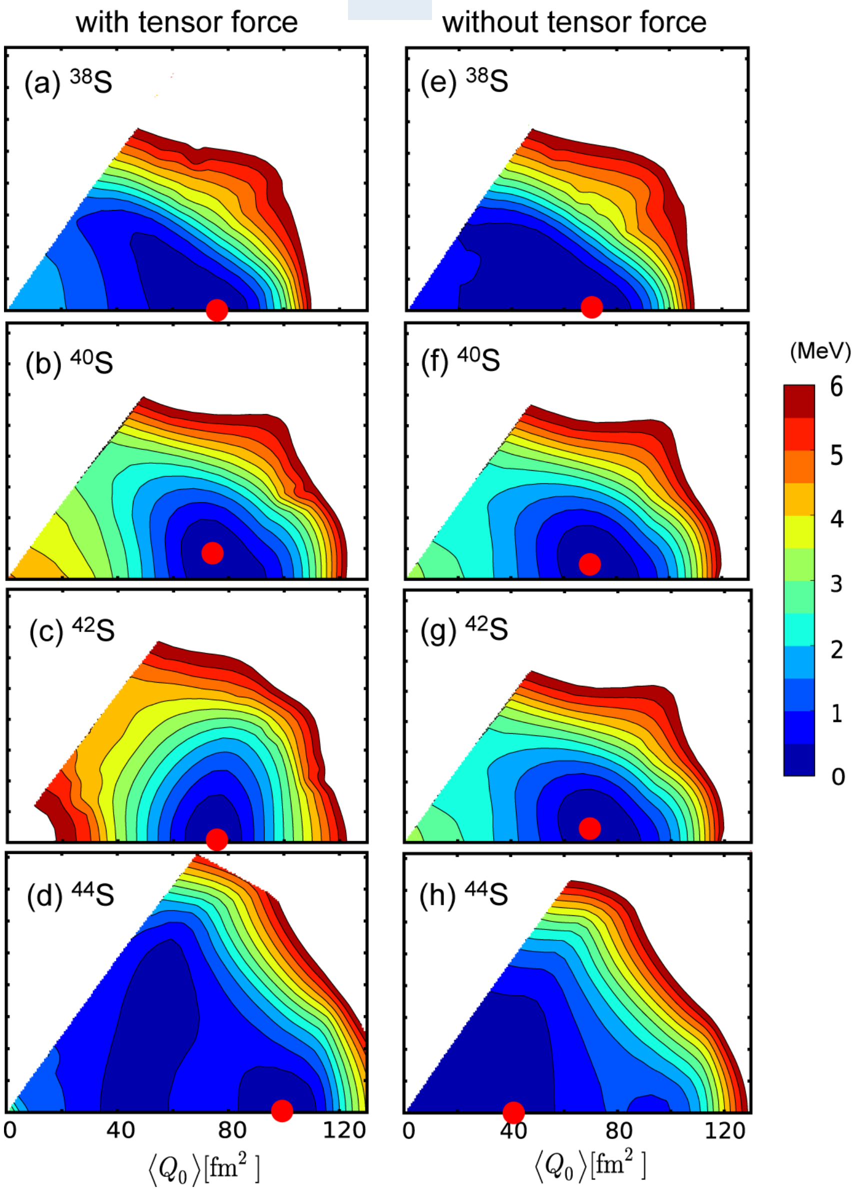
– – – without it

Potential Energy Surface

Si



S

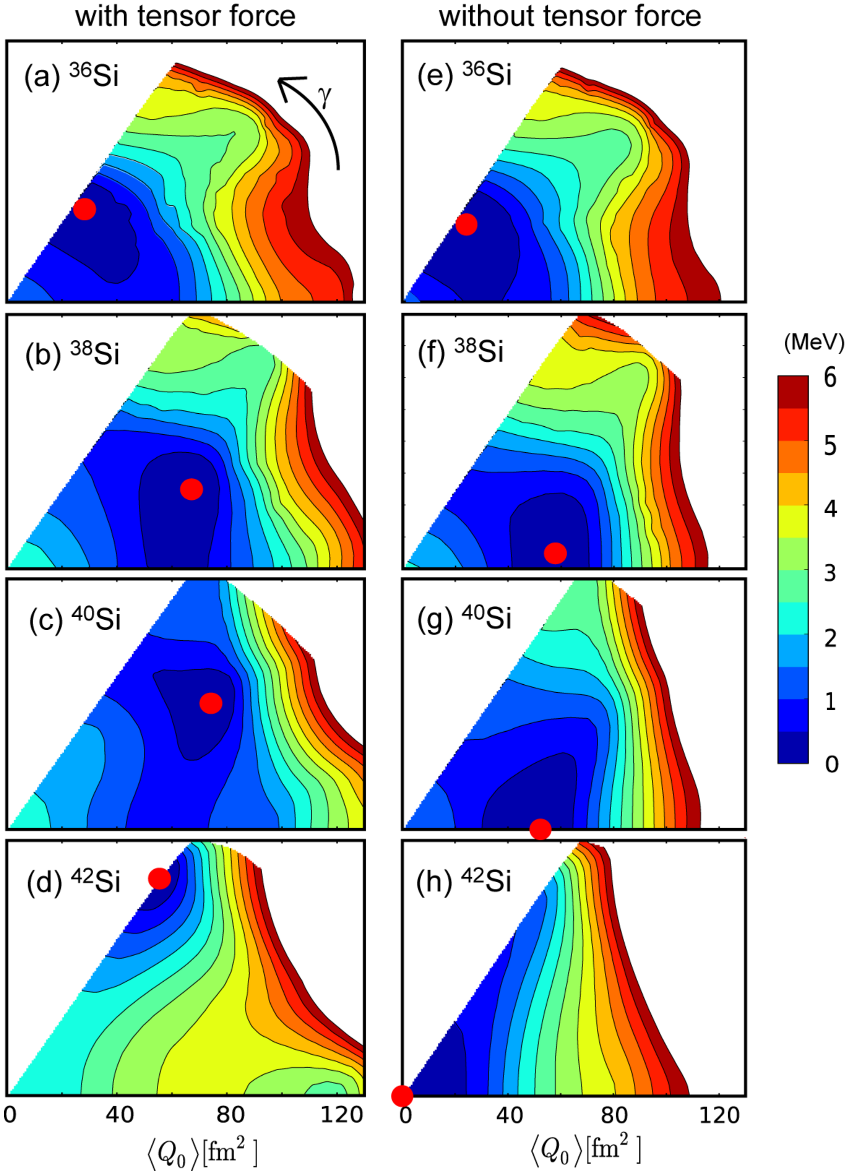


Utsuno, Otsuka, *et al.*, Phys. Rev. C Rapid (2012)

Exotic Si and S isotopes

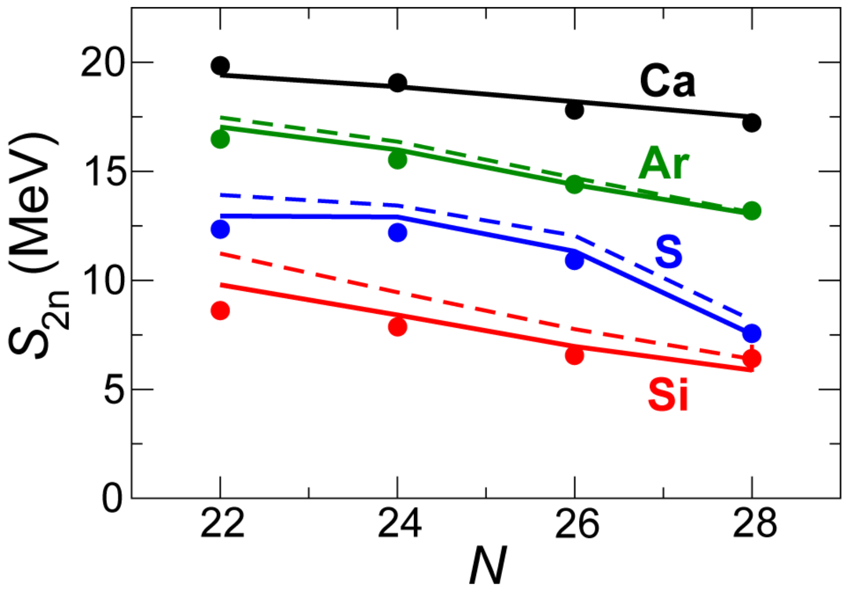
Shapes (PES)

Si



Binding energies

Two-neutron separation energy



—— with cross shell (p-n) tensor force

- - - without it

Utsuno, Otsuka, *et al.*,
Phys. Rev. C Rapid (2012)

Why oblate (or triaxial) favored ?

Underlying robust mechanism ?

In many stable nuclei, $Q_0 > 0$ prolate dominance

A question : Also true for exotic nuclei ?

Primary mean effect of proton – neutron correlation is modeled by

$- f \ Q_0 \text{(proton)} * Q_0 \text{(neutron)}$

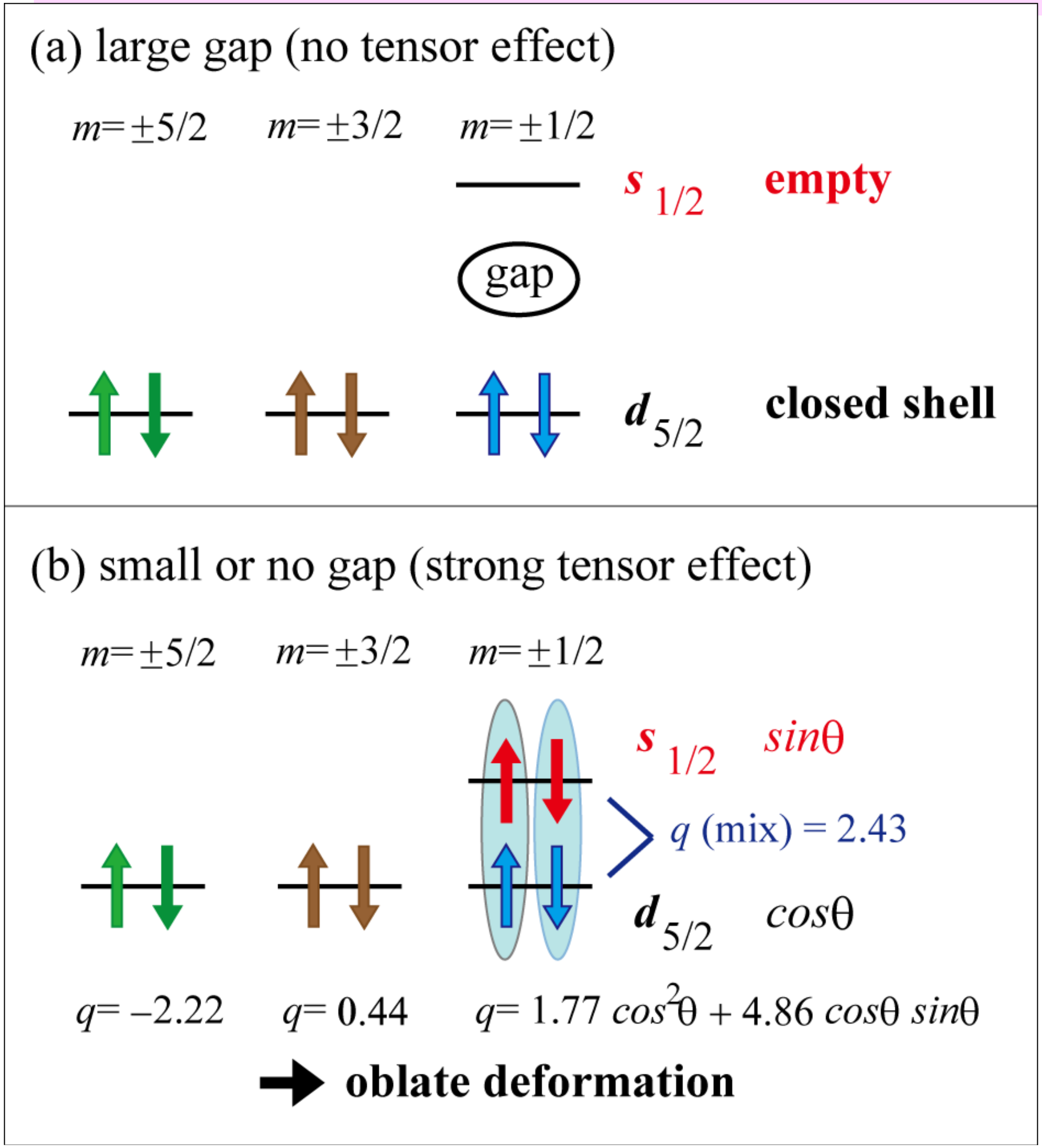
Q_0 : quadrupole moment

$\text{Max} \{Q_0 \text{(proton)} * Q_0 \text{(neutron)} \}$

→ shape of ground state

Why oblate deformation in ^{42}Si ground state ?

Proton wave function of intrinsic state with axial symmetry



(a) large gap (no tensor effect)

(b) small or no gap (strong tensor effect)

→ **oblate deformation**

Spherical magic

$Q_0 = 0$

Oblate shape

intrinsic quadrupole moment

$$Q_0 = 2 \{ q\,(m=5/2) + q\,(m=3/2) + \cos^2\theta \;\; q\,(m=1/2) \} + 4 \cos\theta \; \sin\theta \; q\,(\text{mix})$$

$\{ \ldots \} < 0$ for $\cos^2\theta < 1$

$|Q_0|$ larger, if $Q_0 < 0$ (oblate)

Underlying robust mechanism ?

For ^{42}Si, maximum correlation energy is gained with

Q_0 (proton) < 0, Q_0 (neutron) < 0

both oblate

This is a robust phenomenon for mid-shell nuclei

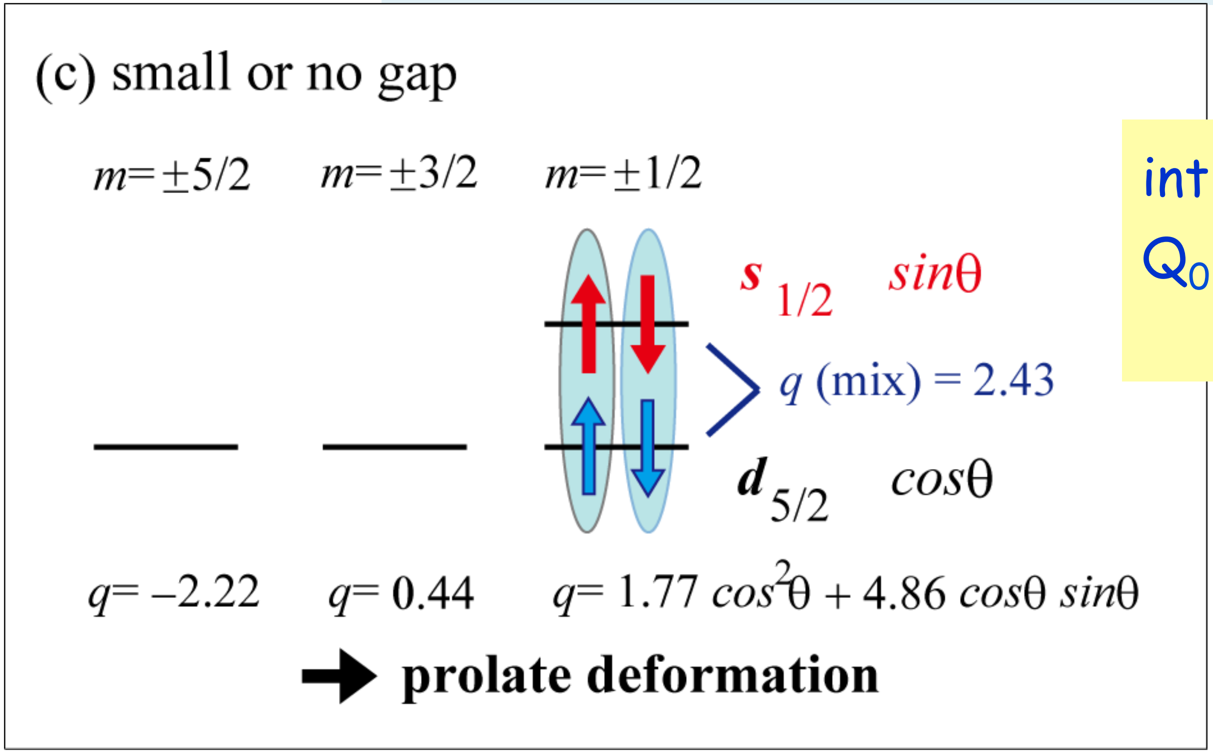
at sub-shell closures with smaller gaps ^{78}**Ni** ?

If the nucleus is at the beginning of the shell, prolate shape is favored (see next slide).

Why prolate deformation at the beginning of the shell ?

Proton wave function of intrinsic state with axial symmetry

mixing by deformed field enhanced by smaller gap



intrinsic quadrupole moment

$$Q_0 = 2\cos^2\theta\ q\,(m=1/2) + 4\cos\theta\sin\theta\ q\,(\text{mix})$$

$|Q_0|$ larger for prolate ($Q_0 > 0$)

like ^{20}Ne