Priority Issue 9
to be Tackled by Using Post K Computer
"Elucidation of the Fundamental Laws and
Evolution of the Universe" (hp160211, hp150224)
KAKENHI grand 25870168

Tsukuba-CCS-RIKEN Workshop
@ Tsukuba CCS 2016/12/15

Nuclear structure and excitations by large-scale shell model calculations

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Contents

- Overview of the Tokyo nuclear theory group on large-scale shell model calculations
  - Zr isotopes by Monte Carlo shell model
  - no-core Monte Carlo shell model + JISP16
  - 4-particle 4-hole excited band around ^{40}Ca
  - Island of inversion by fully microscopic interaction

- Stochastic estimation of level density in large-scale shell model calculations (LSSM)
  - numerical framework of the stochastic estimation of level density
  - application : parity equilibration of ^{58}Ni level density

Computational science projects in Japan

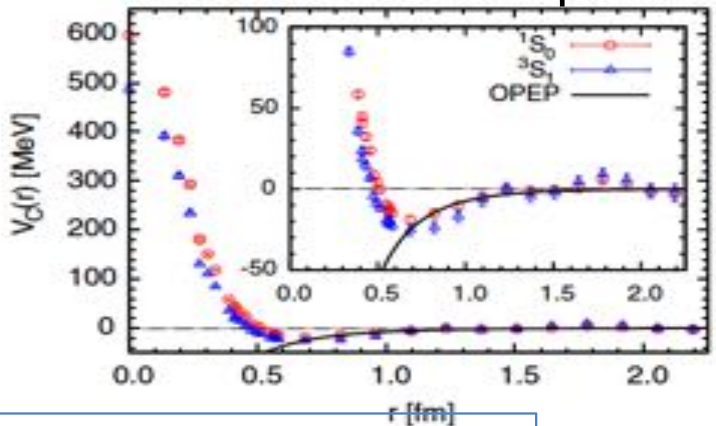
- 9 projects
  – 1st : medicine design
  – …
  – 8th: manufacturing
  – 9th: fundamental science
    - particle physics, nuclear physics, astrophysics, …

JICFuS

"K computer" launched in 2012

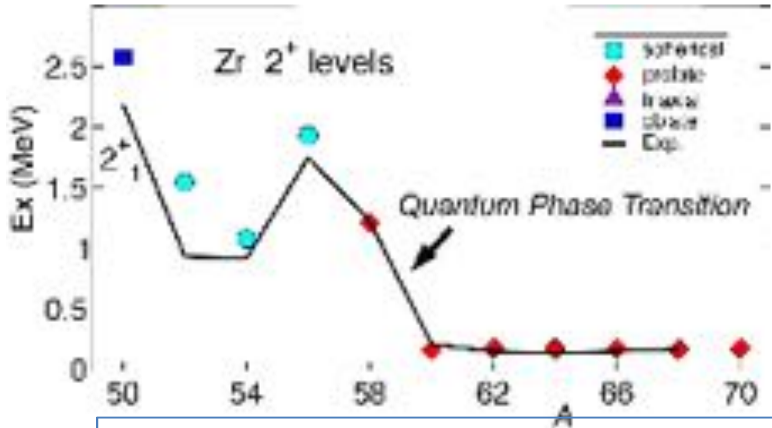
Post-K project in 2021

Hadrons : Lattice QCD calculation to derive the potential



Talks by Aoki, Doi, Iritani

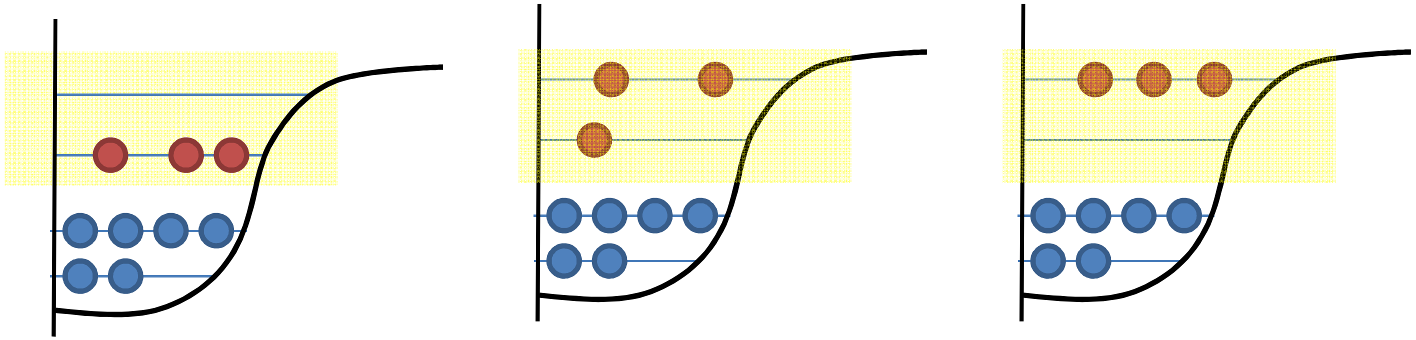
Nuclear structure : LSSM calc. for exotic nuclei



Talks by Otsuka, Shimizu, Menendez

Configurations in nuclear shell model calculation

- Shell-model wave function



$$|\Psi\rangle = v_1|m_1\rangle + v_2|m_2\rangle + v_3|m_3\rangle + \cdots$$

Combinatorial explosion
Feasible up to ~ O(10^{11}) configurations

Schrodinger equation

$$H|\Psi\rangle = E|\Psi\rangle \qquad |\Psi\rangle = \sum_m v_m|m\rangle$$

solve eigenvalue problem of large sparse matrix

Numerical calculations by Lanczos method

$$\sum_{m'} \langle m|H|m'\rangle v_{m'} = E v_m$$

Trend of LSSM calc. and MCSM: M-scheme dimension vs. year

LSSM calc. requires a huge amount of configuration space

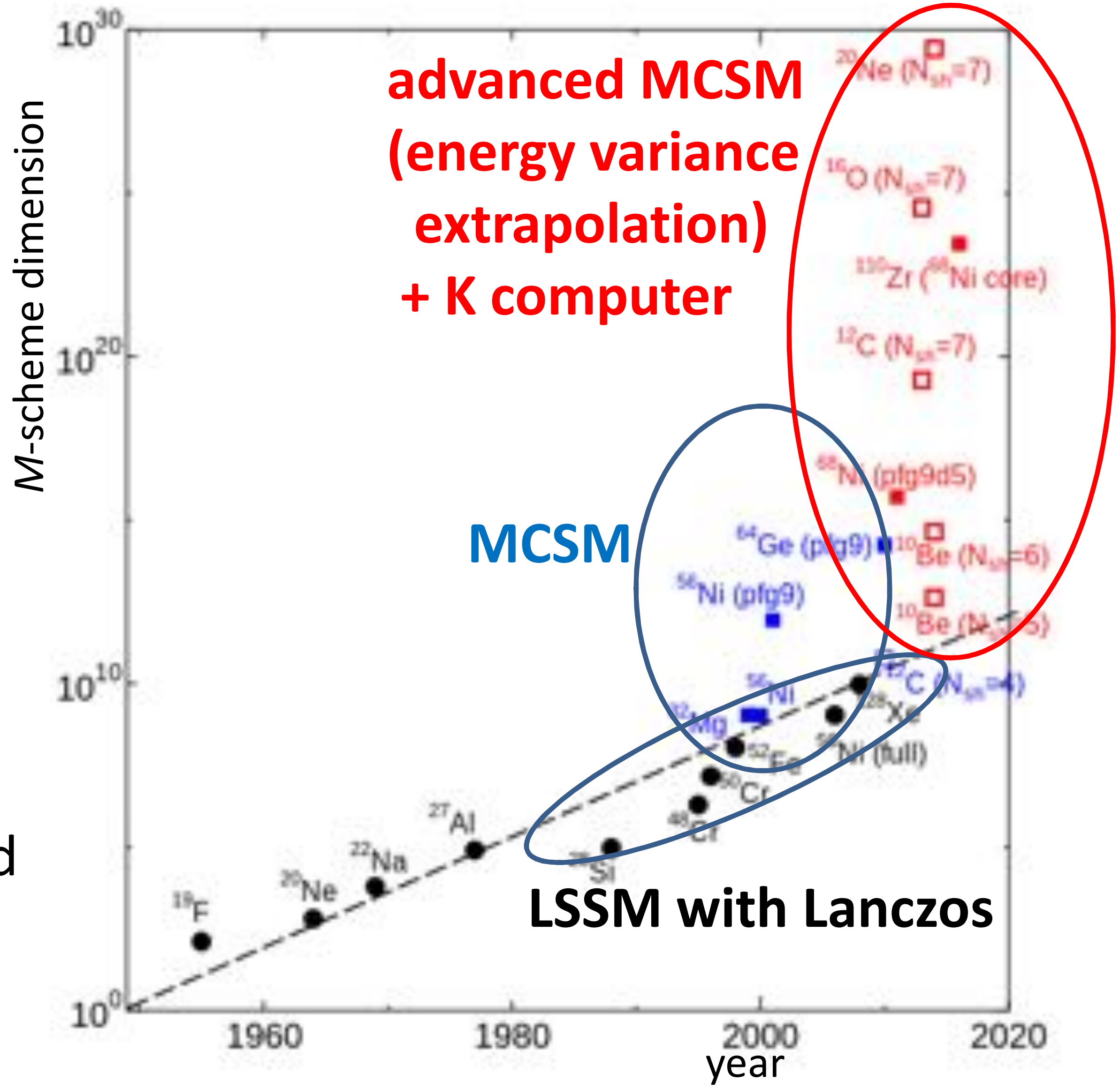
Our strategy :

$$D > 10^{11}$$

Monte Carlo shell model

$$D < 10^{11}$$

LSSM with Lanczos method



Monte Carlo shell model (MCSM)

- Efficient description of nuclear many-body states based on the basic picture of nuclear structure
  = intrinsic state + rotation + superposition

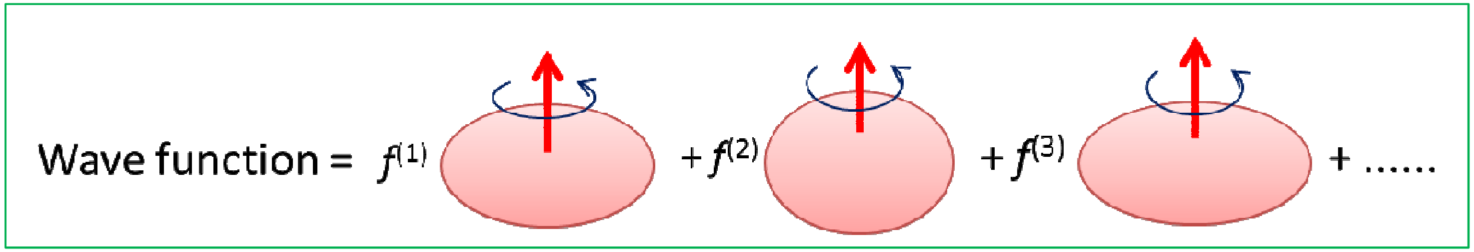
$$|\Psi^{IM\pi}(N_b)\rangle = \underbrace{\sum_{d=1}^{N_b} f^{(d)}}_{\text{superposition}} \underbrace{\sum_{K=-I}^{I} g_K^{(d)} \; \hat{P}^{\pi} \, \hat{P}^{I}_{MK}}_{\text{projection onto good quantum numbers}} \underbrace{|\Phi(D^{(d)})\rangle}_{\text{optimized Slater determinant}}$$

MCSM basis dimension ≈ 100

superposition → mixing with different shapes

projection onto good quantum numbers → rotation

optimized Slater determinant → deformed intrinsic state

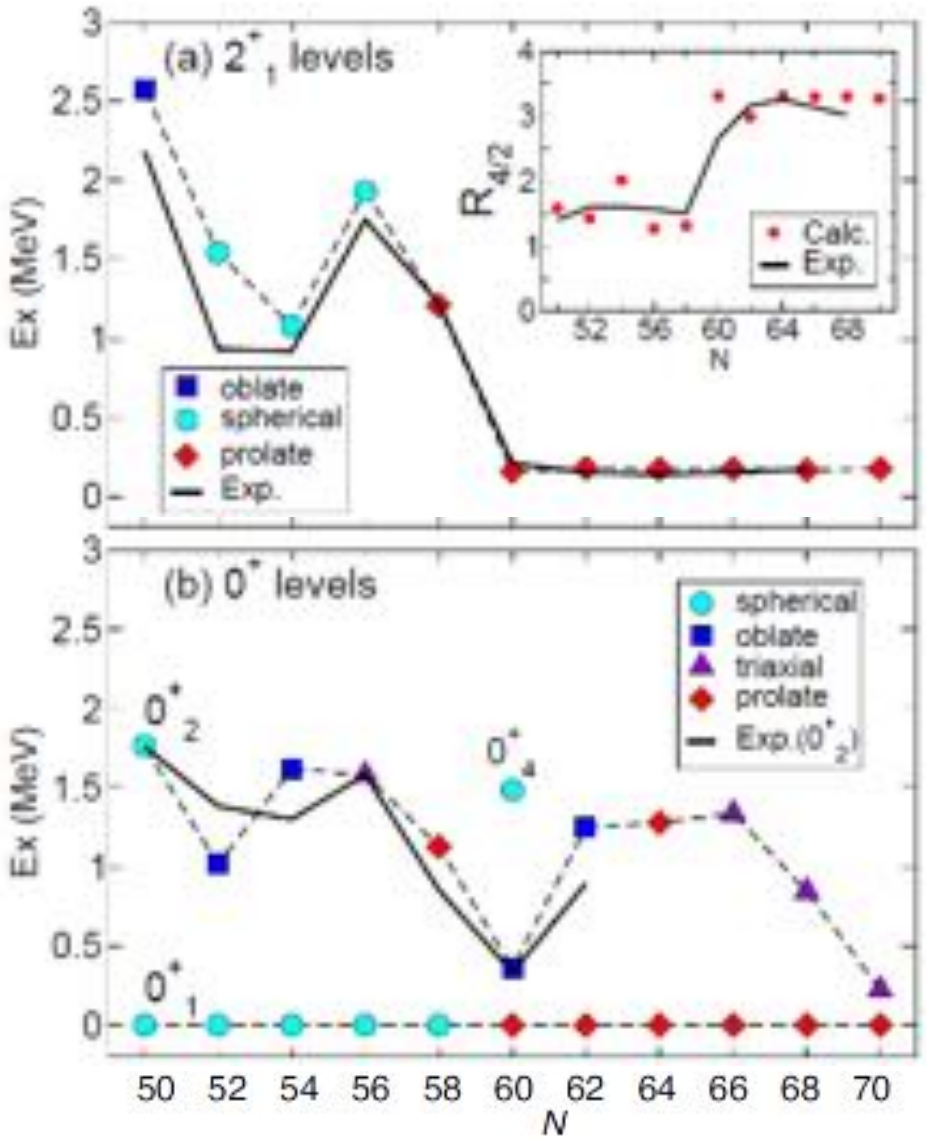


$f^{(d)}$, $g_K^{(d)}$, $D^{(d)}$: variational parameters determined to minimize $\langle \Psi^{IM\pi}|H|\Psi^{IM\pi}\rangle$
variation after J^{π}-projection and superposition

Extrapolation using energy variance is applied

Recent achievement:
Quantum Phase Transition in the Shape of Zr isotopes

T. Togashi *et al.*, PRL 117, 172502 (2016)



drastic change of Ex(2^+) at N=60

"quantum phase transition" from spherical to prolate deformation is shown by the analysis of Monte Carlo shell model (model space: 28<Z<70, 40<N<94, realistic effective int.)

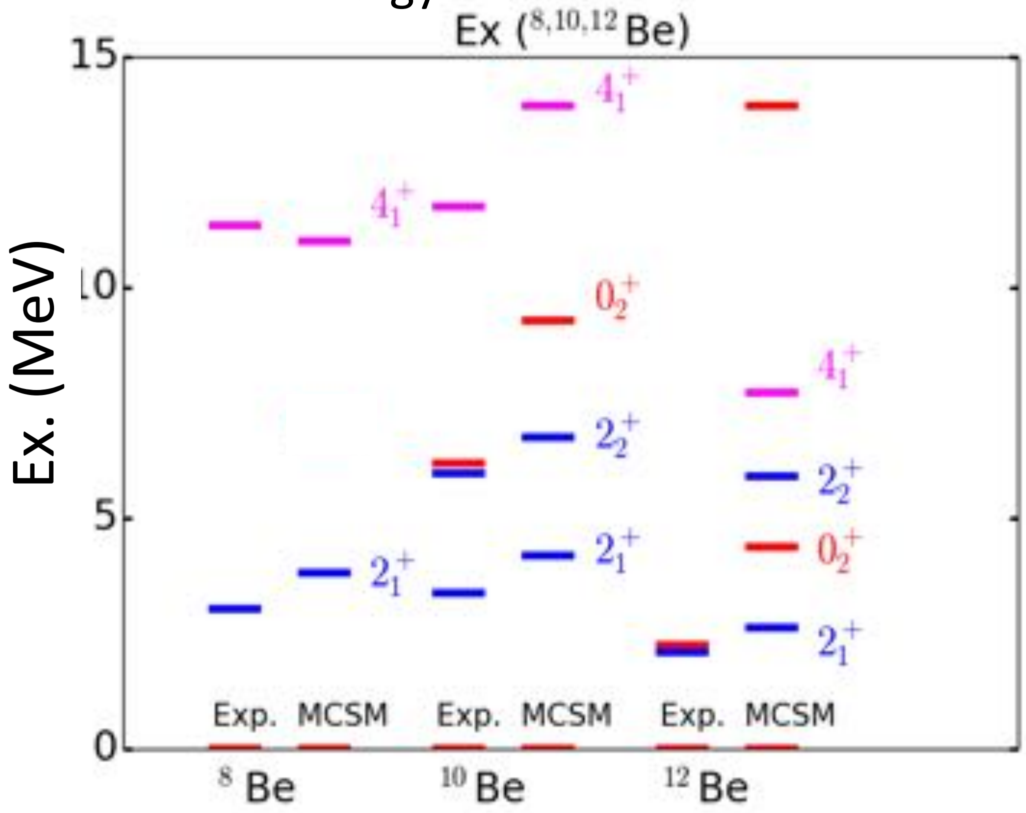
"Quantum Self-Organization"

Ref. Talk by Takaharu Otsuka (Tuesday)

T. Yoshida, N. Shimizu, T Abe and T. Otsuka

No-core Monte Carlo shell model + JISP16

Energy levels of ^{8,10,12}Be



Expt. ^{8}Be,^{10}Be: Tilley *et al*., 2004,
^{12}Be: Shimoura *et al.*, 2003

No-core shell-model calculations with

$N_{\rm shell} = 6, \quad \hbar\omega = 15$ MeV

JISP16 interaction

The overall tendency is rather good, whereas excitation energies are somewhat overestimated.

T. Yoshida, N. Shimizu, T Abe and T. Otsuka

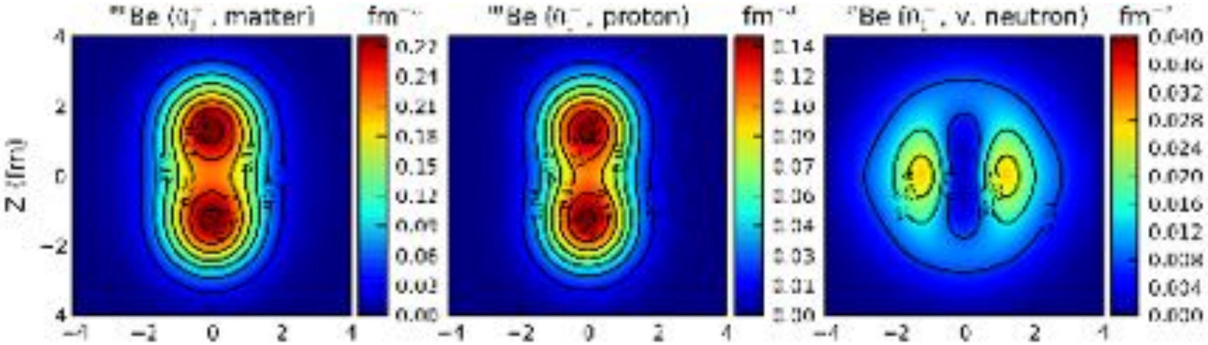
Intrinsic density by Monte Carlo shell model : Molecular orbits in ^{10}Be

Matter

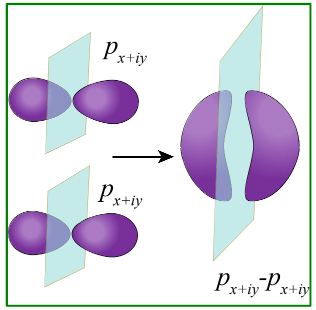
Proton

Valence neutron (neutron – proton)

^{10}Be 0_1^+

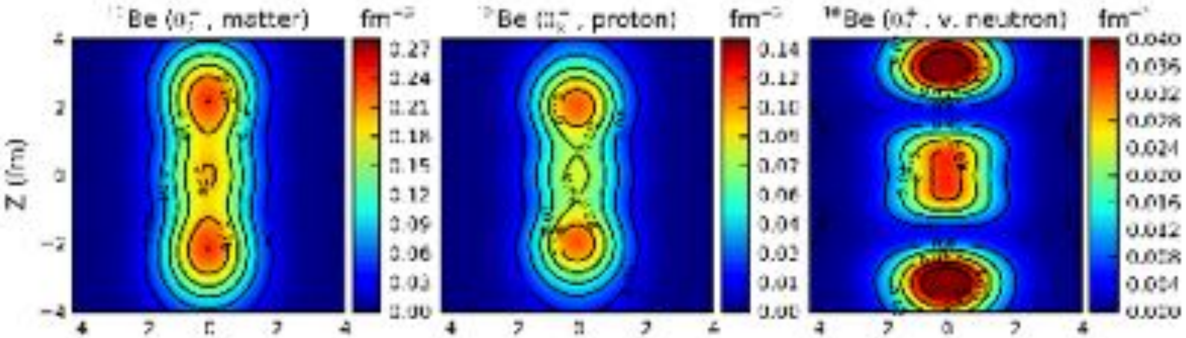


Pi molecular orbit

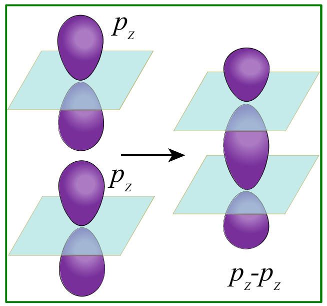


Excited state

^{10}Be 0_2^+



Sigma molecular orbit



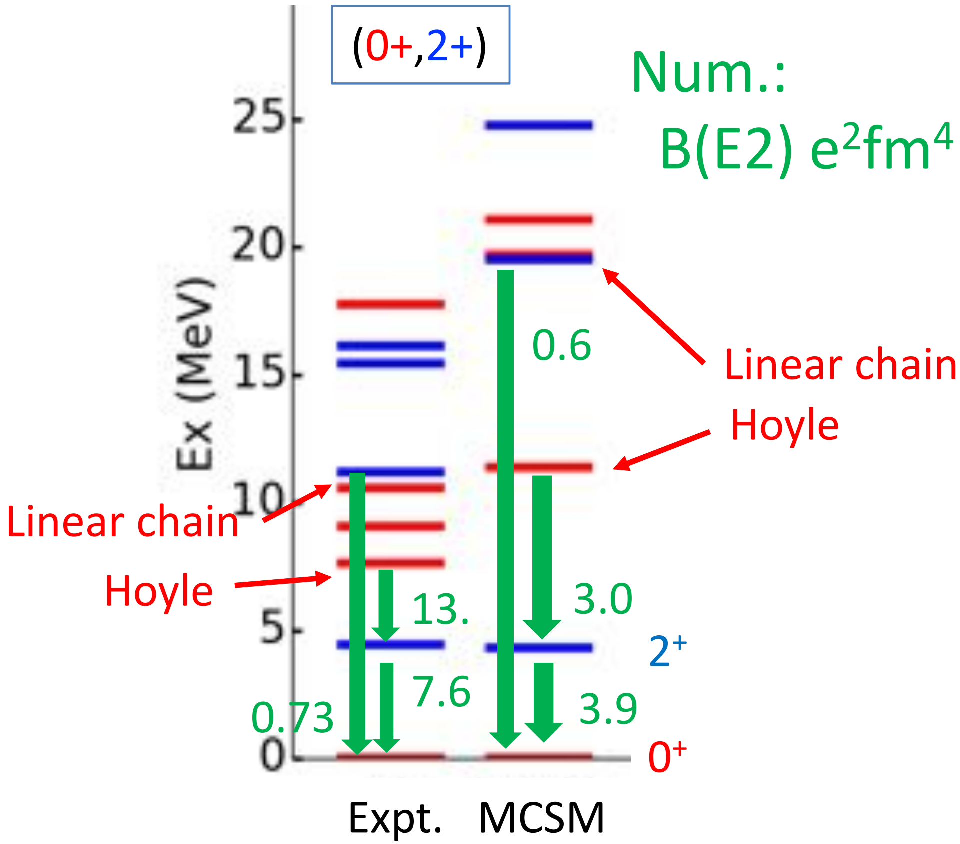
Elongation effect for 2-alpha distance

Appearance of sigma molecular orbit

T. Yoshida, N. Shimizu, T Abe and T. Otsuka

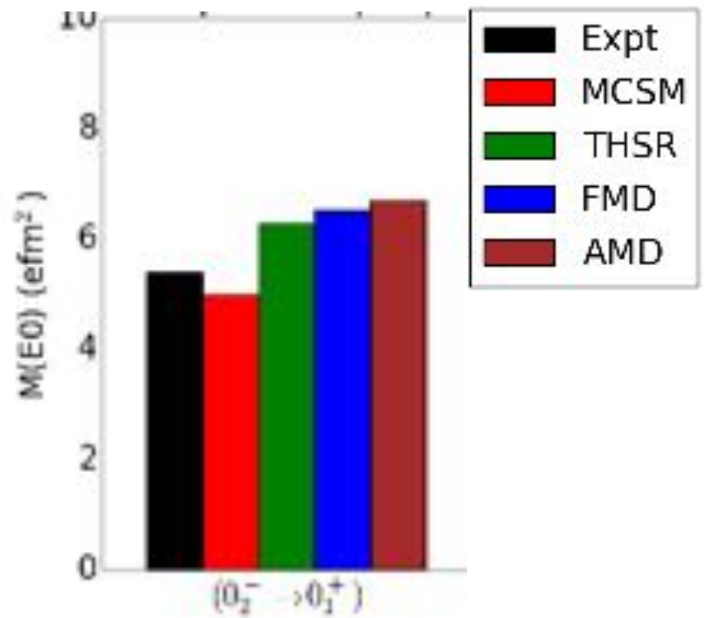
^{12}C by no-core Monte Carlo shell model

JISP16 interaction
model space : 6 H.O. major shells



Expt: M. Itoh et al PRC84 (2011)
MCSM: $N_{\mathrm{shell}} = 6, \quad \hbar\omega = 15$ MeV

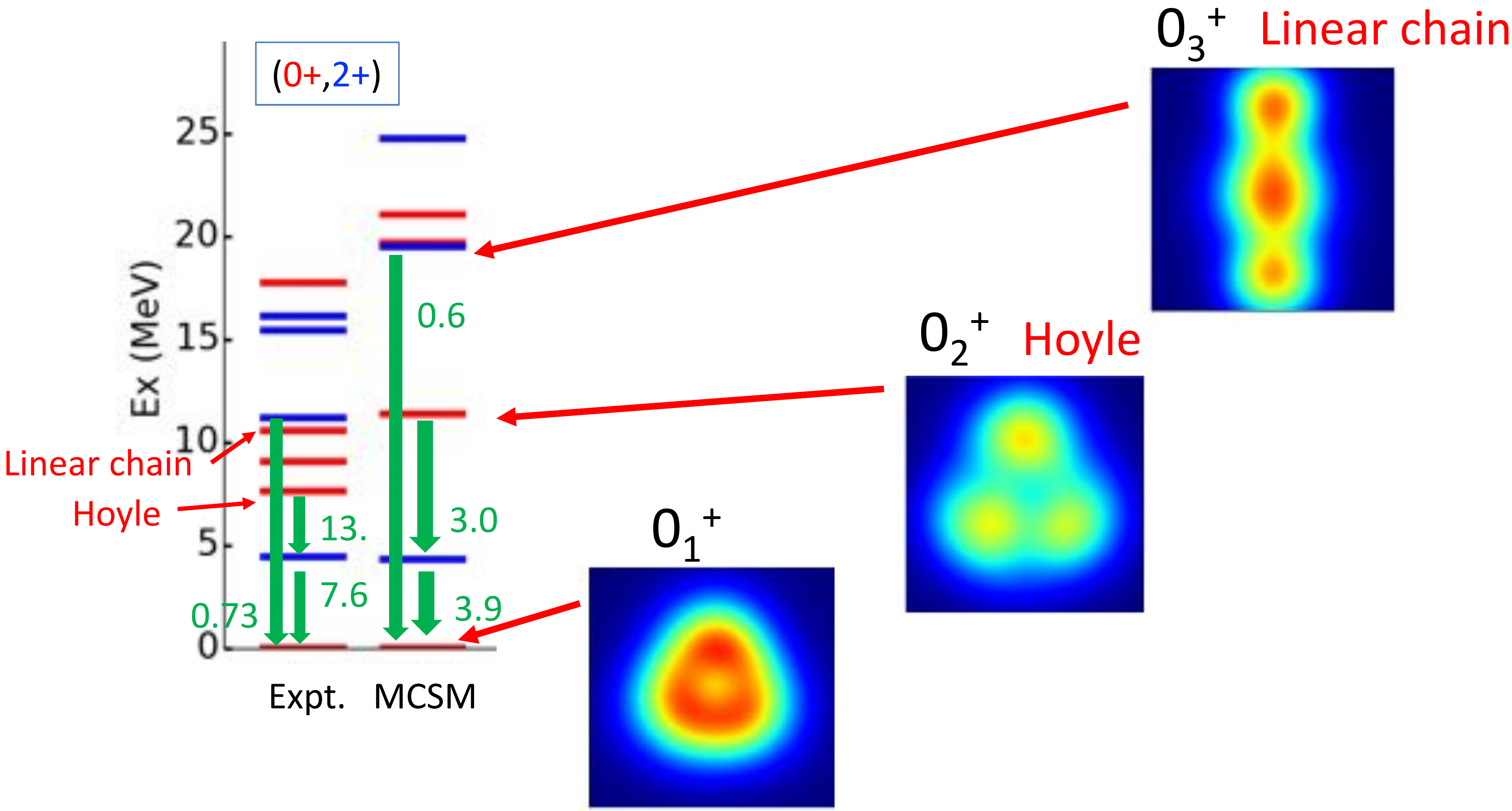
$$M(E0; 0_2^+ \longrightarrow 0_1^+)$$



Expt.: P. Strehl 1970
THSR: Y. Funaki 2015
FMD: M. Chernykth 2007
AMD: Y. Kanada-En'yo 2007

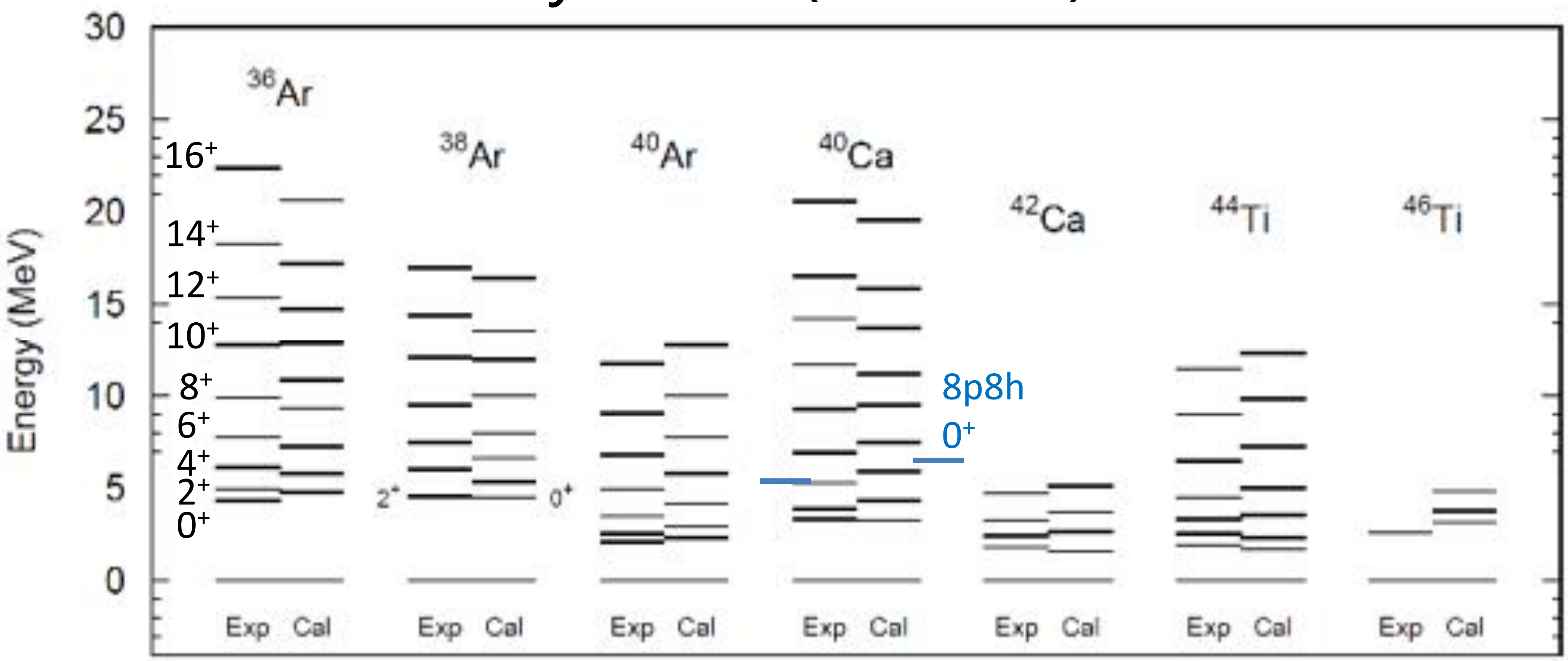
T. Yoshida, N. Shimizu, T Abe and T. Otsuka

Density profile of the MCSM wave function of $^{12}C\ 0^+$ states



T. Ichikawa *et al.*

4-particle 4-hole excited bands around ^{40}Ca by LSSM (Lanczos)

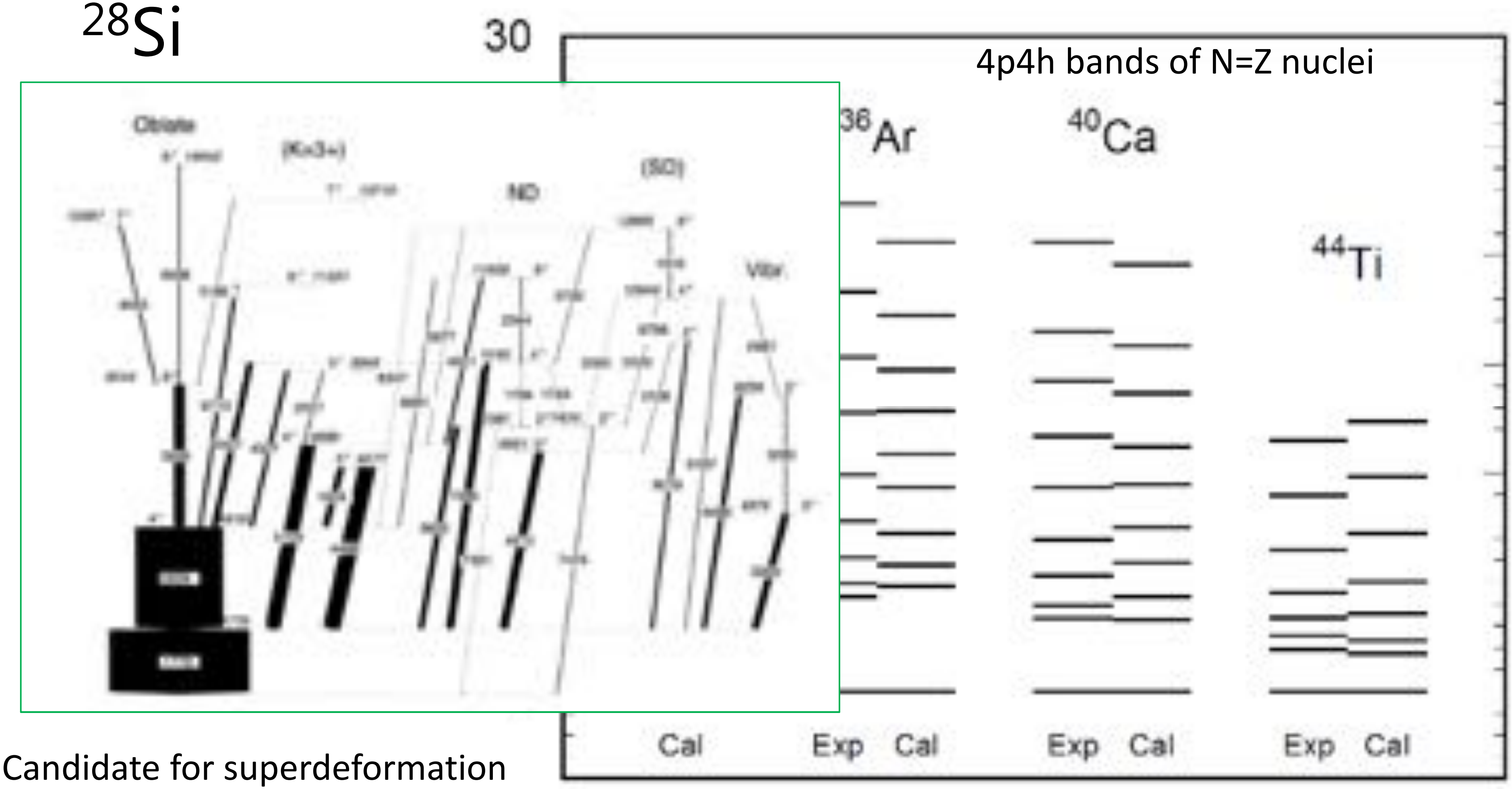


- model space : *sd*-shell, *f*7/2, *p*3/2
- SDPF-M interaction with minor modification
- maximum M-scheme dimension reaches 6.6 x 10^{10}

T. Ichikawa *et al.*

^{28}Si superdeformed band ?

^{28}Si



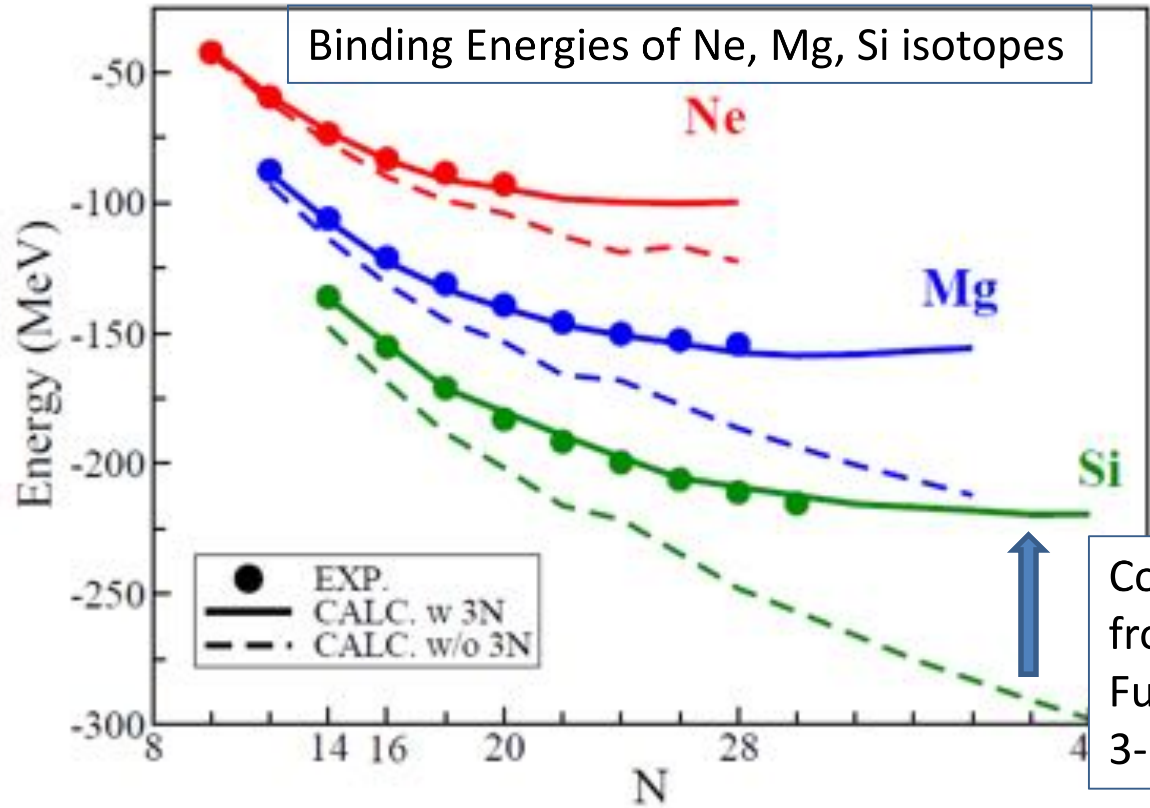
Candidate for superdeformation
Jenkins 2012, based on Taniguchi 2009

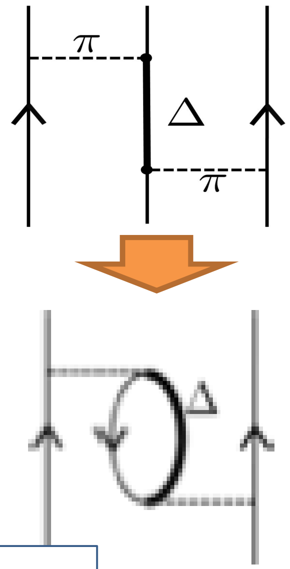
No 4p4h state of ^{28}Si is found in LSSM (preliminary)

Microscopic derivation of effective interaction in medium-heavy nuclei

N. Tsunoda *et al.*, arXiv:1601.06442

Binding Energies of Ne, Mg, Si isotopes





Contribution from Fujita-Miyazawa 3-body force

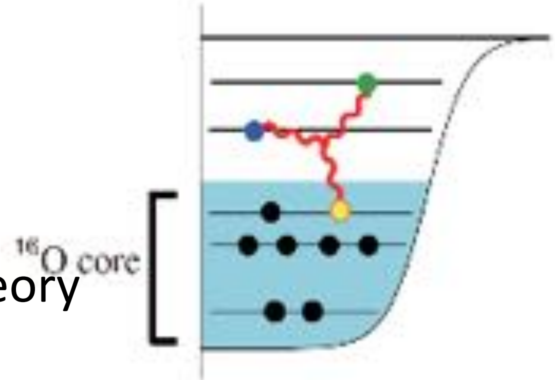
“Island of inversion” by LSSM with *sdpf*-shells

Effective interaction with phenomenological correction

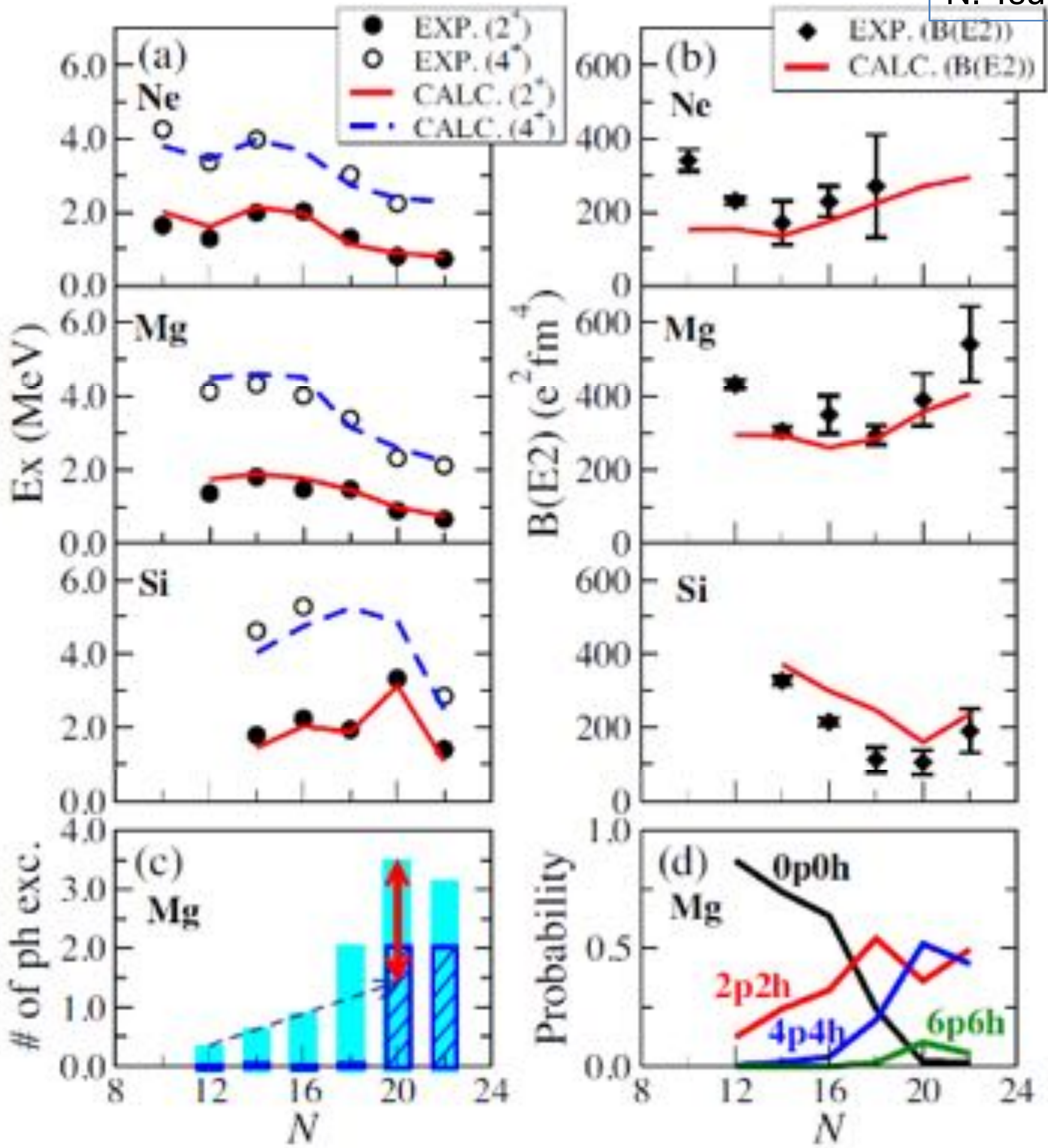
⇒ microscopic derivation

from sophisticated many-body perturbation (EKK) theory

+ Fujita-Miyazawa three-body force



N. Tsunoda *et al.*, arXiv:1601.06442



Effective charges

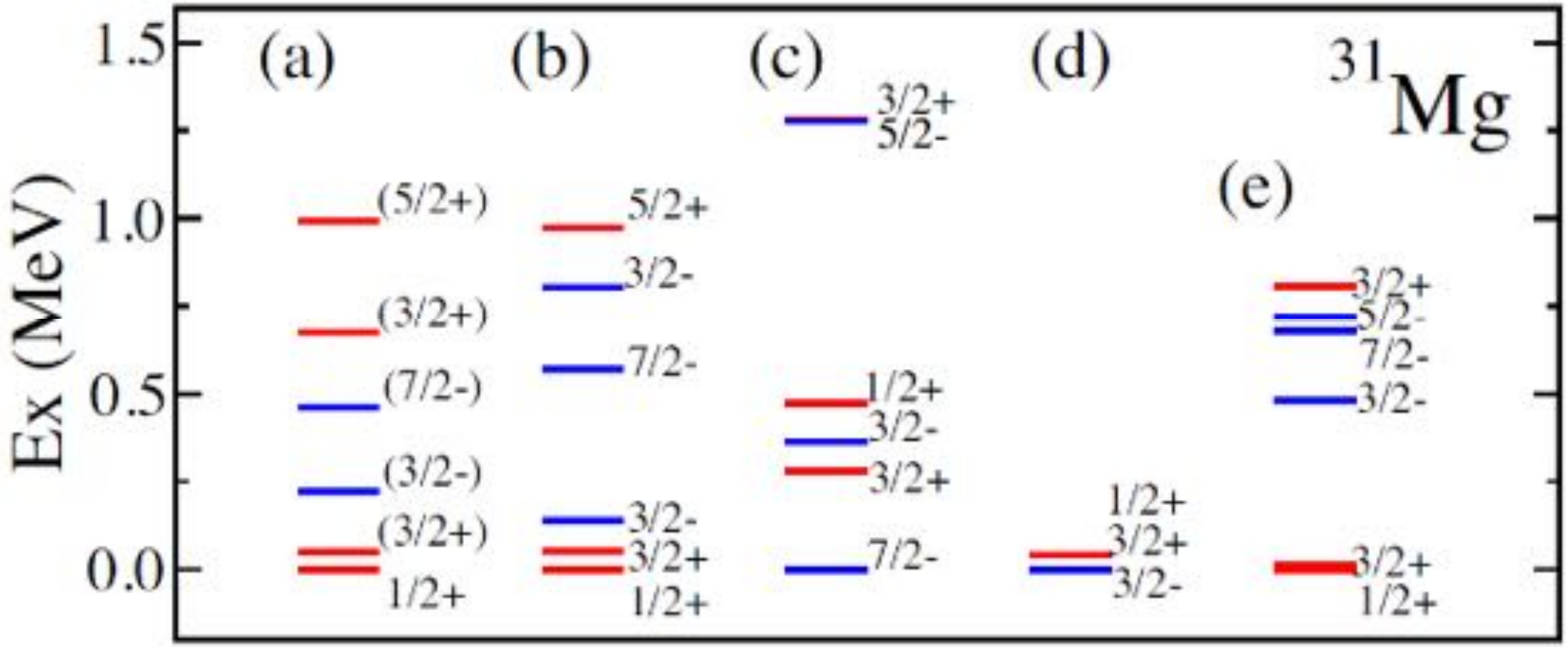
(ep,en)=(1.25, 0.25)

- Clear indication of breaking of N=20 gap for Ne and Mg.
- N=20 gap remains in Si case.

N. Tsunoda *et al.*, arXiv:1601.06442

^{31}Mg levels by EKK + 3NF

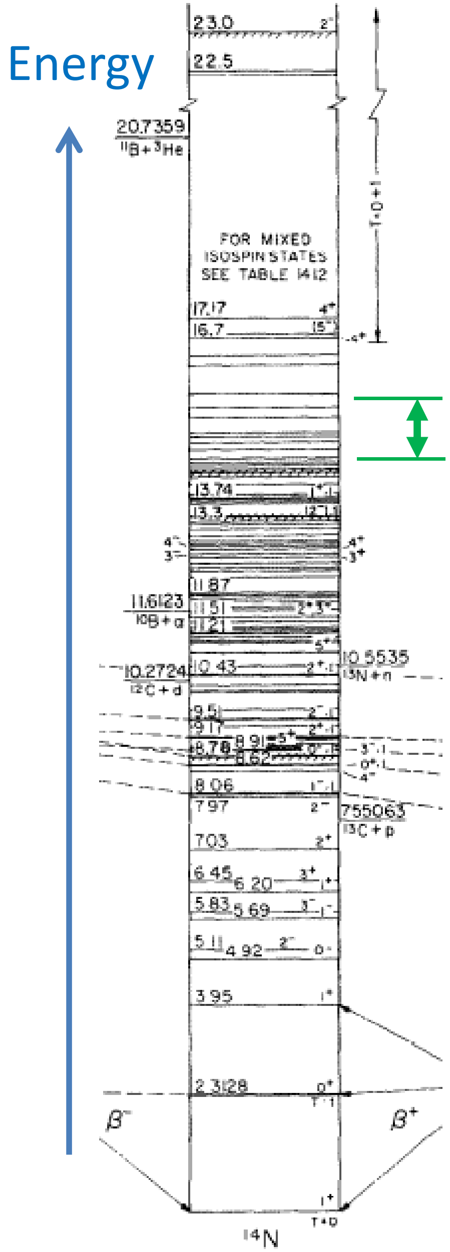
Exp. present SDPF-M sdpf-u-mix AMD+GCM



Stochastic estimation of nuclear level density in the nuclear shell model: An application to parity-dependent level density in ^{58}Ni

Noritaka Shimizu (U. Tokyo), Yutaka Utsuno (JAEA),
Yasunori Futamura (U. Tsukuba), Tetsuya Sakurai (U. Tsukuba),
Takahiro Mizusaki (U. Senshu), and Takaharu Otsuka (U. Tokyo)
Phys. Lett. B **753**, 13 (2016)

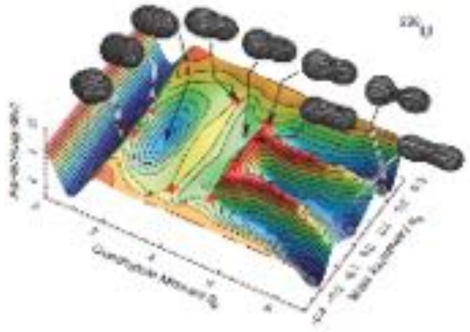
Nuclear level density

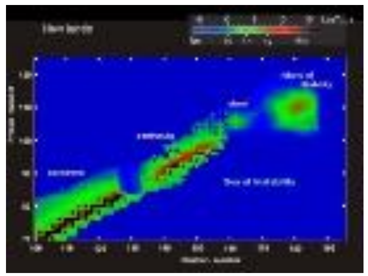


- Statistical model is important where the level density is large

- Hauser-Feshbach theory
  - input: Level density, γ-ray strength function, optical potential
  - output: neutron-capture cross section

Nuclear engineering





Nucleosynthesis

superheavy nuclei

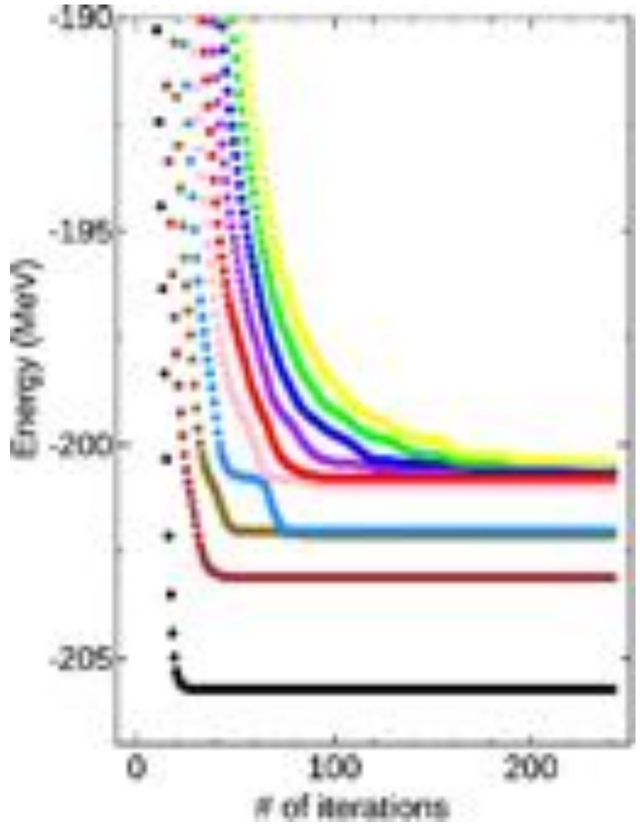
Nuclear level density in LSSM

- Level density is a key input for Hauser-Feshbach theory. An empirical formula is usually used to obtain the level density.
  ⇒ microscopic model wanted

- Nuclear shell-model calculation is one of the most powerful tools to describe level density including various many-body correlations.

- Shell Model Monte Carlo (Y. Alhassid, H. Nakada *et al.*) is a most powerful tool to estimate level density. However, "sign problem" prevents us from using general realistic interaction.

- We propose a novel efficient method to compute level density in shell-model calculations avoiding direct count.



Convergence of eigenvalues in conventional Lanczos method (^{56}Ni, pf-shell)
Difficult to obtain highly-excited high-density region

Level density in nuclear shell-model calc.

- Level density ⇒ count the number of eigenvalues of huge sparse matrix in a certain energy region

JSIAM Letters Vol.2 (2010) pp.127–130 ©2010 Japan Society for Industrial and Applied Mathematics JSIAM Letters

Parallel stochastic estimation method of eigenvalue distribution

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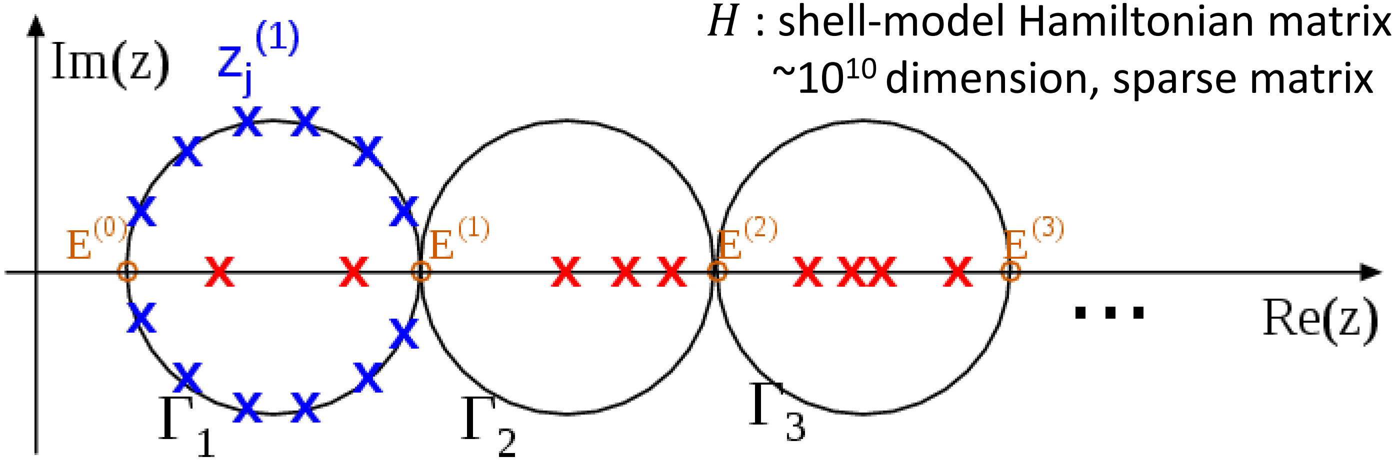
Received July 29, 2010, Accepted October 22, 2010

Tool to compute eigenvalue distribution of huge sparse matrix with contour integral + shifted conjugate gradient method

Counting eigenvalues : Cauchy integral

Count poles of $f(z) = \mathrm{Tr}\left((z-H)^{-1}\right) = \sum_i \frac{1}{z-E_i}$

H : shell-model Hamiltonian matrix in *M*-scheme
~10^{10} dimension, sparse matrix



$$\mu_k = \frac{1}{2\pi i}\oint_{\Gamma_k} dz\ \mathrm{tr}((z-H)^{-1})$$

$$\simeq \sum_j w_j \boxed{\mathrm{tr}((z_j^{(k)}-H)^{-1}),}$$

discretize

Next step : Stochastic estimation of trace

Hutchinson estimator

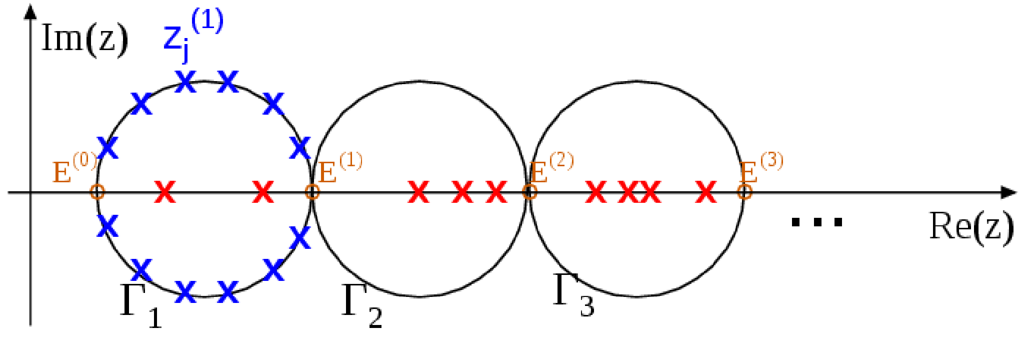
Estimate the matrix trace in Monte Carlo way

$$\mathrm{Tr}(A) \cong \frac{1}{N_s}\sum_{i=1}^{N_s} v_i^T A v_i$$

- matrix elements of the vector, v_i , are taken as -1 or 1 randomly with equal probability.
- well known in applied mathematics
- statistical error is small if non-diagonal matrix elements of A are small. (exact if A is diagonal)
- $v_i^T A v_i \ = \mathrm{Tr}(A) + \underbrace{\sum_{k \neq k'} (v_i)_k A_{kk'} (v_i)_{k'}}_{\text{Statistical error : non-diagonal part}}$

Ref. M. F. Hutchinson, Comm. Stat. Sim. **19**, 433 (1990)

Stochastic estimation of “trace”



$$\mathrm{Tr}\left((z-H)^{-1}\right)=\sum_i \frac{1}{z-E_i}$$

$$\mu_k = \oint_{\Gamma_k} \mathrm{tr}\left((z\text{-}H)^{-1}\right)dz$$

D: Whole dimension

- estimating $\mathrm{tr}(z-H)^{-1}$

$$=\sum_i^{\boxed{D}} \boldsymbol{e}_i^T (z-H)^{-1}\boldsymbol{e}_i$$

N_s: Number of samples

- Stochastic sampling

$$\simeq \frac{1}{N_s}\sum_s^{\boxed{N_s}} \boxed{\boldsymbol{v}_i^T (z-H)^{-1}\boldsymbol{v}_i}$$

N_s=32 show Next step : Matrix inverse

$\boldsymbol{v}_i^T (z - H)^{-1} \boldsymbol{v}_i$

⇒ solve linear equations to avoid the inverse of matrix

solve $\boldsymbol{v}_i = (z - H)\, \boldsymbol{x}_i$ and obtain $\boldsymbol{v}_i^T \boldsymbol{x}_i$

$\boldsymbol{v}_i = A\, \boldsymbol{x}_i$

Complex Orthogonal Conjugate Gradient (COCG)

$$
\begin{aligned}
x_{k+1} &= x_k + \alpha_k p_k, \\
r_{k+1} &= r_k - \alpha_k \boxed{A p_k}, \\
p_{k+1} &= r_{k+1} + \beta_k p_k,
\end{aligned}
$$

$$\alpha_k = r_k^T r_k / p_k^T A p_k$$

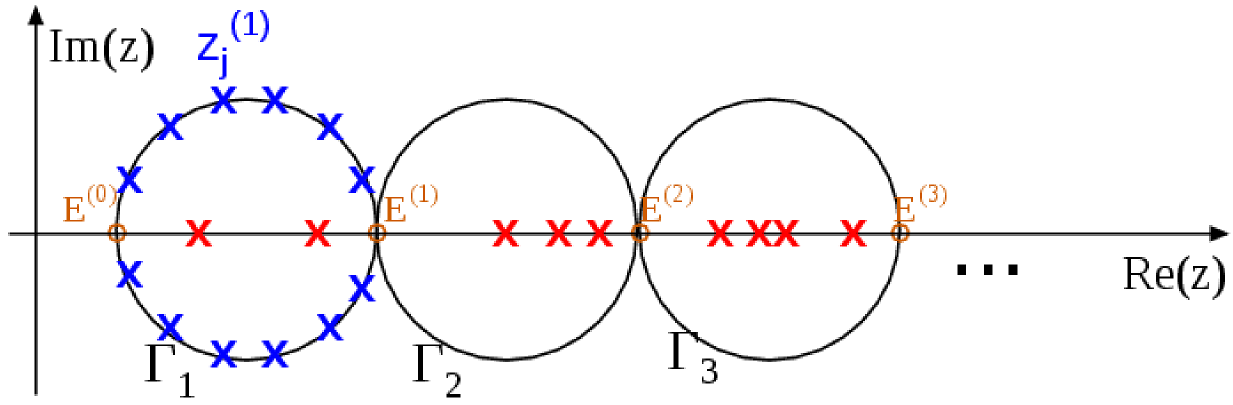
$$\beta_k = r_{k+1}^T r_{k+1} / r_k^T r_k$$

The matrix appears only in matrix-vector product

⇒ efficient for sparse matrix

In practice, we adopt Block COCG (BCOCG) with block bilinear form.

Introduction to shift algorithm



too many $z_j^{(i)}$ to be computed ...

$\Rightarrow$ Shift algorithm

solve $\boldsymbol{v}_i = (z_{ref} - \sigma - H)\,\boldsymbol{x}_i$ σ: shift

using solution of solve $\boldsymbol{v}_i = (z_{ref} - H)\,\boldsymbol{x}_i$

Shift invariance of Krylov subspace

- Purpose : solve $A\boldsymbol{x} = \boldsymbol{b}$ and $(A - \sigma)\boldsymbol{x} = \boldsymbol{b}$ simultaneously

  (σ: constant number, "shift")
- Krylov subspace

$$\mathcal{K}r(A, b) = \{b, Ab, A^2b, A^3b, \dots, A^{n-1}b\}$$

- COCG solution of$A\boldsymbol{x} = b$ is always on the Krylov subspace
- Is the solution of $(A - \sigma)\boldsymbol{x} = b$?

  $\Rightarrow$ It is on the same Krylov subspace

$$\begin{aligned}\mathcal{K}r(A - \sigma, b) &= \{b, (A - \sigma)b, (A - \sigma)^2 b, \dots, (A - \sigma)^{n-1}b\} \\ &= \mathcal{K}r(A, b)\end{aligned}$$

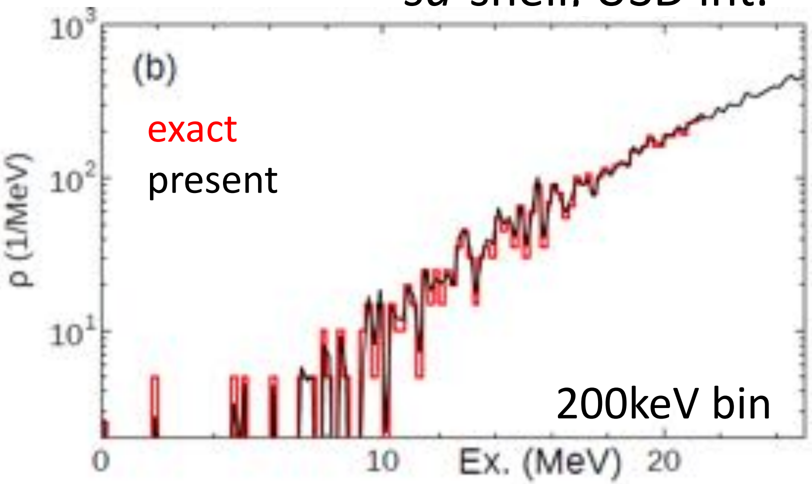
- Especially in COCG method, the residual of the shifted COCG is conserved except for its norm

$$r_k^\sigma = \frac{1}{\pi_k^\sigma} r_k$$

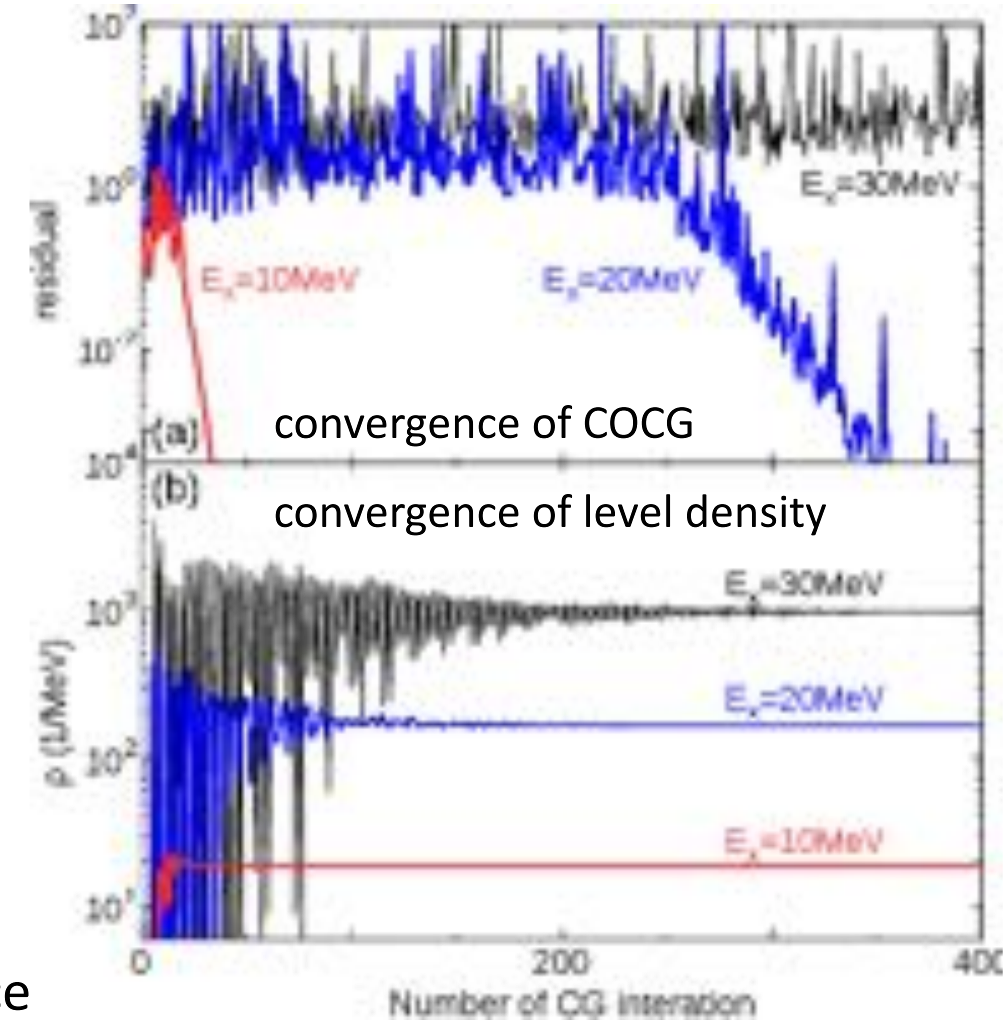
$$\begin{aligned}\pi_{k+1}^\sigma &= (1 + \alpha_k \sigma)\pi_k^\sigma + \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}}(\pi_k^\sigma - \pi_{k-1}^\sigma), \\ \alpha_k^\sigma &= \frac{\pi_k^\sigma}{\pi_{k+1}^\sigma}\alpha_k, \\ \beta_k^\sigma &= \left(\frac{\pi_k^\sigma}{\pi_{k+1}^\sigma}\right)\beta_k\end{aligned}$$

Benchmark test

Exact vs. stochastic estimate (N_s=32) for the level density in ^{28}Si *sd*-shell. USD int.



Stochastic estimation well reproduces the exact value!

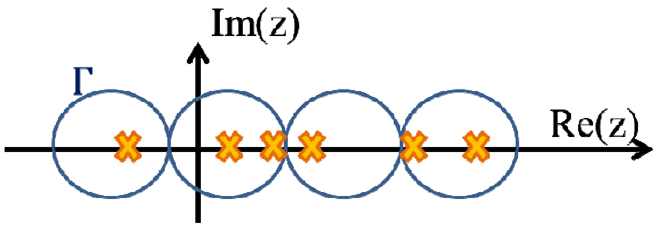


- High excitation energy
  ⇒ high level density
  ⇒ slow COCG convergence
- Level density converges much faster than COCG

Level density by large-scale shell model calc.

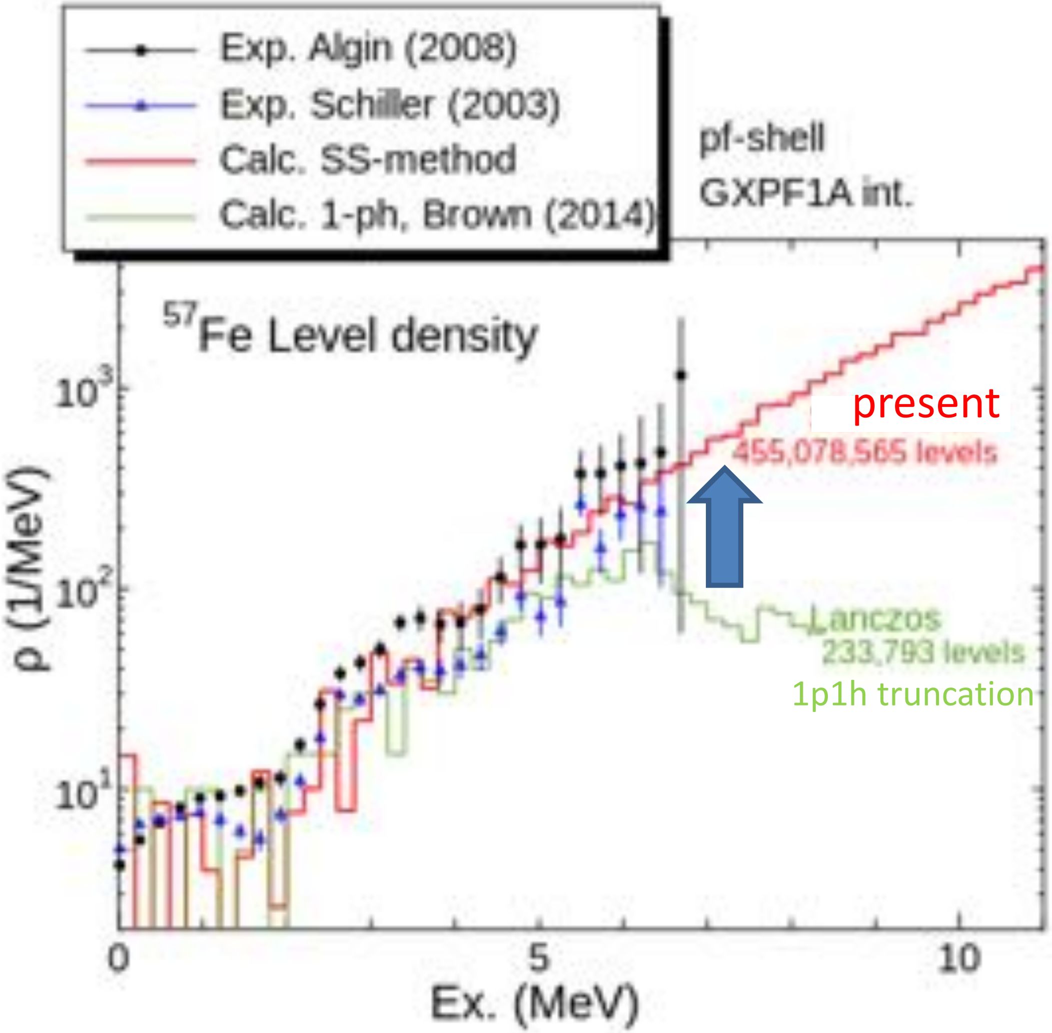
Stochastic estimation for density of states

$$\rho(E) = \oint_\Gamma \mathrm{tr}\left((z\text{-}H)^{-1}\right) dz$$



$$\rho(E) \approx \frac{1}{N} \sum_i \oint_\Gamma \vec{v}_i (z\text{-}H)^{-1} \vec{v}_i \, dz$$

$$\approx \frac{1}{N} \sum_{i,j} w_j \vec{v}_i (z_j\text{-}H)^{-1} \vec{v}_i$$



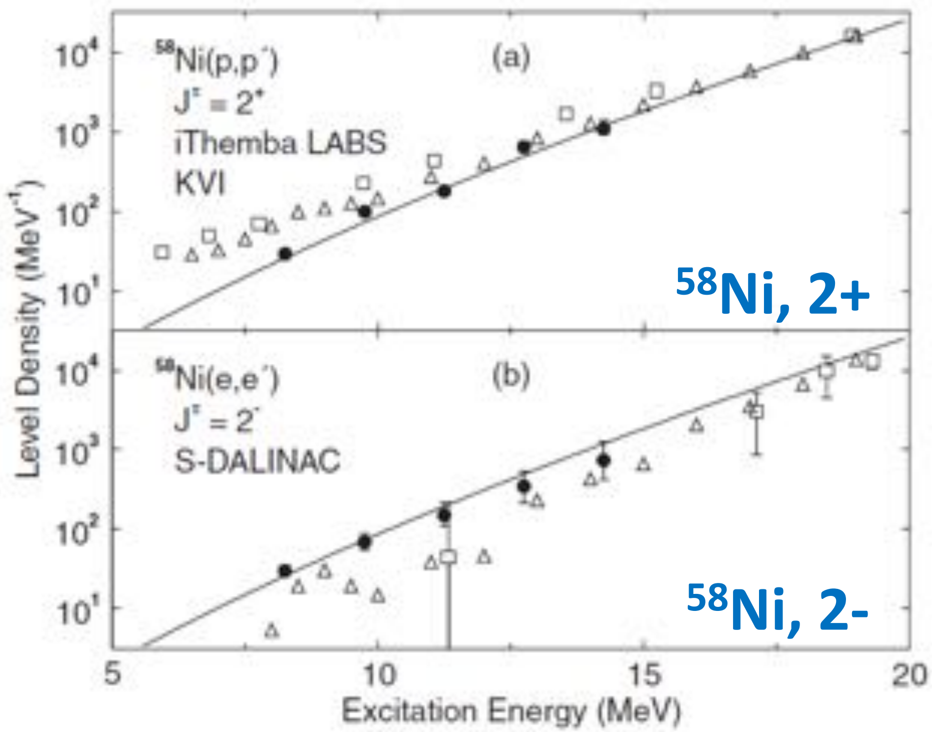
SM calc. with realistic interaction provides us with a good description of level density

Puzzle: parity dependence of level density

- Spin-parity dependence:
  crucial for application (due to selectivity)

● experiment
□ SMMC
△ HFB

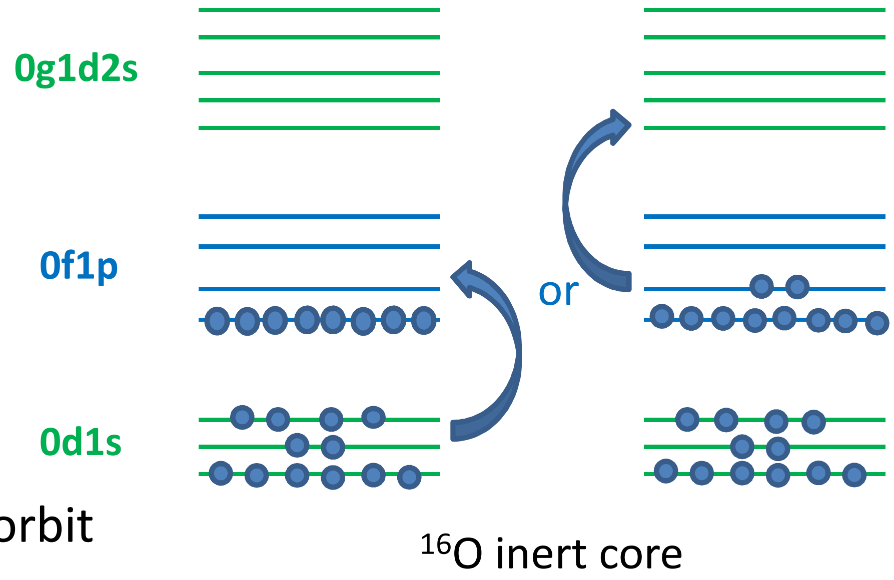
- Parity-equilibration of level density is often assumed by empirical formulas
- Experiment shows that 2+ and 2- level densities of ^{58}Ni are similar value to each other (Kalmykov 2007)
- Microscopic calculations (SMMC, HFB-based methods) overestimate 2+ level density and underestimate 2- level density



Ref. Y. Kalmykov, C. Ozen, K. Langanke, G. Martinez-Pinedo, P. von Neumann-Cosel and A. Richter, Phys. Rev. Lett. **99**, 202502 (2007).

Model space and interaction for LSSM calc. of *pf* -shell nuclei

- Target :
  - *pf*-shell nuclei (e.g. Ni isotopes)
- Valence shell
  - Full *sd-pf-sdg* shell
  - $0\hbar\omega$ for natural-parity states and
    $1\hbar\omega$ states for unnatural-parity states
  - up to 6-particle excitation from $0f_{7/2}$ orbit



- Effective interaction
  - SDPF-MU for *sd, pf* shells VMU for *sdg* shell (Y. Utsuno 2012)
    - SDPF-MU is successful in *sd-pf* shell calculations including exotic nuclei (e.g. ^{42}Si, ^{44}S)
  - $g_{9/2}$ SPE: fitted to $9/2^+_1$ in ^{51}Ti
- Removal of spurious center-of-mass motion
  - Lawson method: $H = H_{SM} + \beta H_{CM}$

Large-scale shell model calculations around ^{58}Ni

- Excitation energies and one-particle spectroscopic factors around ^{58}Ni

- Model space :
  - *sd, pf, sdg* shells
  - SDPF-MU for *sd, pf* shells VMU for *sdg* shell
  - 0ħω for natural-parity states, 1ħω for unnatural-parity states
  - up to 6-particle excitation from $0f_{7/2}$ orbit
  - 1.5×10^{10} *M*-scheme dim. for ^{58}Ni 2^- states

Nucl.	J^π	E_x (MeV) Cal.	E_x (MeV) Exp.	C^2S j	C^2S Cal.	C^2S Exp.
^{57}Co	$7/2_1^-$	0	0	$\pi 0f_{7/2}^{-1}$	5.28	4.27, 5.53
^{58}Ni -p	$1/2_1^+$	3.037	2.981	$\pi 1s_{1/2}^{-1}$	0.98	1.05, 1.31
	$3/2_1^+$	3.565	3.560	$\pi 0d_{3/2}^{-1}$	1.70	1.50, 2.33
^{57}Ni	$3/2_1^-$	0	0	$\nu 1p_{3/2}^{-1}$	1.14	1.04, 1.25, 0.96
^{58}Ni -n	$1/2_1^+$	5.581	5.580	$\nu 1s_{1/2}^{-1}$	0.51	0.62, 1.08
	$3/2_1^+$	5.579	4.372	$\nu 0d_{3/2}^{-1}$	0.29	0.01
	$3/2_2^+$	6.093	6.027	$\nu 0d_{3/2}^{-1}$	0.22	0.66, 0.54
^{59}Cu	$3/2_1^-$	0	0	$\pi 1p_{3/2}^{+1}$	0.53	0.46, 0.49, 0.25
^{58}Ni +p	$9/2_1^+$	3.139	3.023	$\pi 0g_{9/2}^{+1}$	0.26	0.24, 0.32, 0.27
^{59}Ni	$3/2_1^-$	0	0	$\nu 1p_{3/2}^{+1}$	0.51	0.82, 0.33
^{58}Ni +n	$9/2_1^+$	3.053	3.054	$\nu 0g_{9/2}^{+1}$	0.63	0.84, 0.39
	$5/2_1^+$	4.088	3.544	$\nu 1d_{5/2}^{+1}$	0.04	0.03
	$5/2_2^+$	4.595	4.506	$\nu 1d_{5/2}^{+1}$	0.30	0.23, 0.14
	$1/2_1^+$	4.399	5.149	$\nu 2s_{1/2}^{+1}$	0.00	0.09
	$1/2_2^+$	5.492	5.569	$\nu 2s_{1/2}^{+1}$	0.18	0.02
	$1/2_3^+$	5.589	5.692	$\nu 2s_{1/2}^{+1}$	0.02	0.13

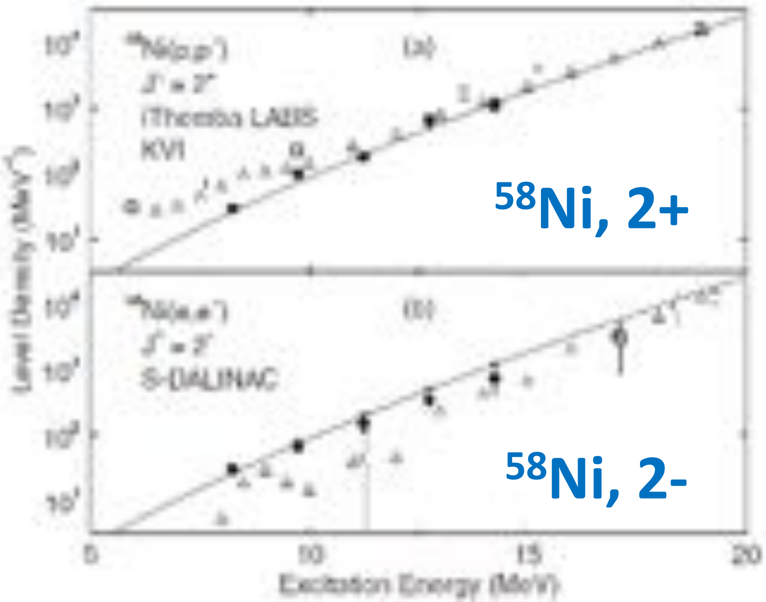
SDPF-MU int. Y. Utsuno *et al.*, PRC 86, 051301R (2012)
VMU int. T. Otsuka *et al.*, PRL 104, 012501 (2010)

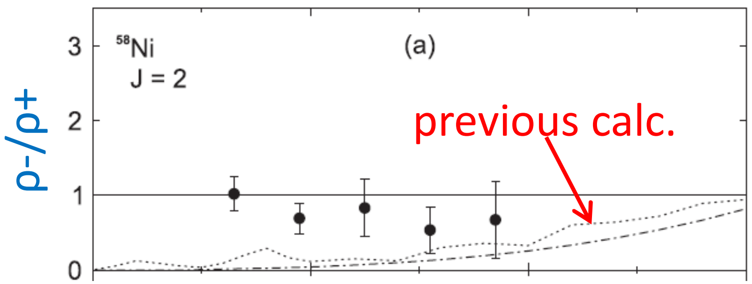
Single-particle characters of 58Ni ±p, n are successfully described by LSSM

Application: parity dependence of level density

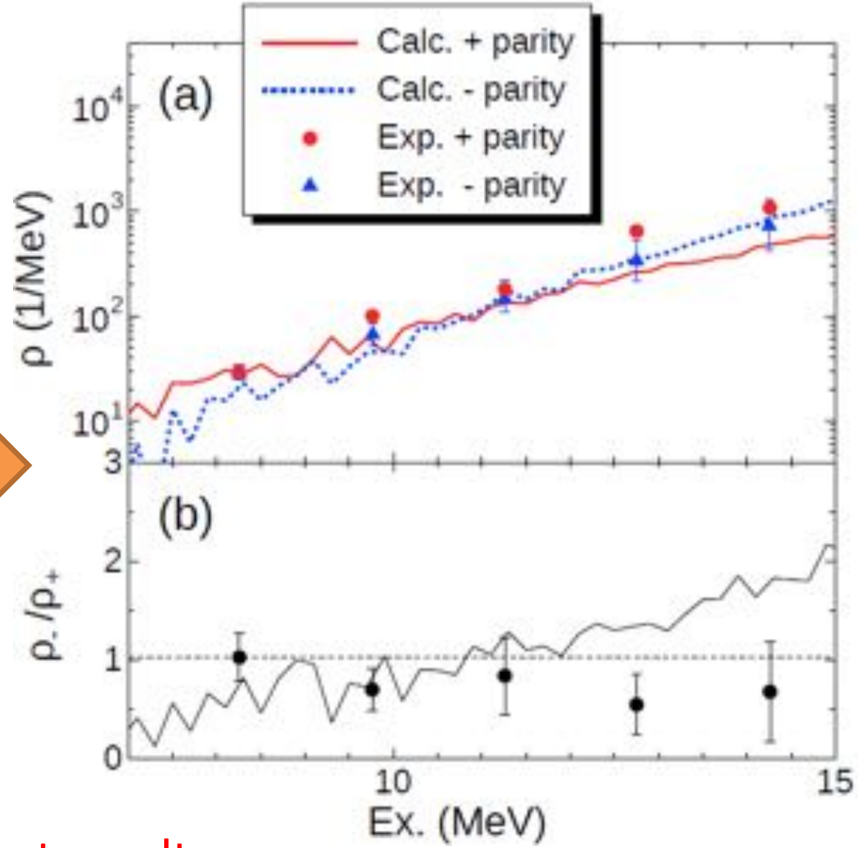
Contradiction between experiment and theory is resolved.

- No parity dependence (exp.) vs. strong parity dependence (prev. calc.)





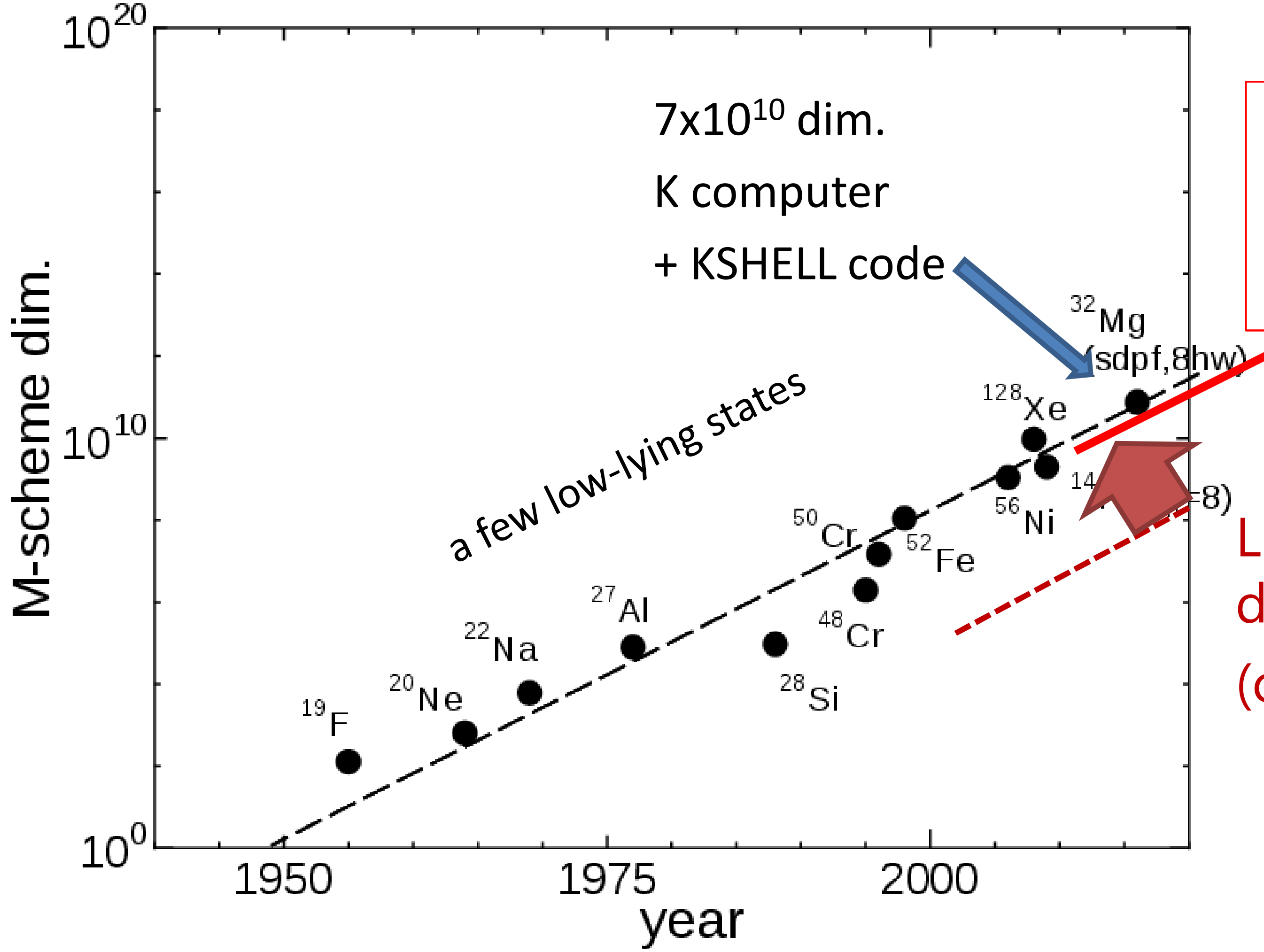
Ref. Y. Kalmykov *et al.*, PRL **99**, 202502 (2007).



Present result

Common setup to the study of exotic nuclei

Current limitation of large-scale shell-model calc.



Limit for stochastic estimation of level density

Limit for level density

(count 1000 states)

Summary

- Under Post-K project, we develop MCSM and LSSM codes for solving nuclear many-body problem
  - no-core MCSM and clustering structures of Be isotopes and ^{12}C
  - 4-particle 4-hole excited bands around ^{40}Ca by LSSM
  - construct fully microscopic interaction to discuss "island of inversion"

- A new stochastic estimation of level density in nuclear shell-model calculations utilizing conjugate gradient method
  - Parity equilibration of ^{58}Ni J=2 states of and low-lying spectroscopic information around ^{58}Ni are successfully described in a shell-model framework