



KAKENHI grand 25870168

Priority Issue 9

to be Tackled by Using Post K Computer

“Elucidation of the Fundamental Laws and
Evolution of the Universe” (hp160211, hp150224)

NTSE 2016 @ Pacific National University,
Khabarovsk, Russia, 2016/09/21

Large-scale shell-model studies for exotic nuclei and nuclear level densities



Noritaka Shimizu
Center for Nuclear Study, the University of Tokyo



Contents

- Introduction of the activities in Tokyo nuclear theory group : large-scale nuclear structure calculations
 - Zr isotopes by Monte Carlo shell model
 - no-core Monte Carlo shell model + JISP16
 - Be isotopes + intrinsic density
 - UMOA + Daejeon 16
- Stochastic estimation of level density in large-scale shell model calculations (LSSM)
 - numerical framework of the stochastic estimation of level density
 - benchmark test
 - application : parity equilibration of ^{58}Ni level density

Computational science projects in Japan

- 9 projects
 - 1st : medicine design
 - ...
 - 8th: manufacturing
 - 9th: fundamental science

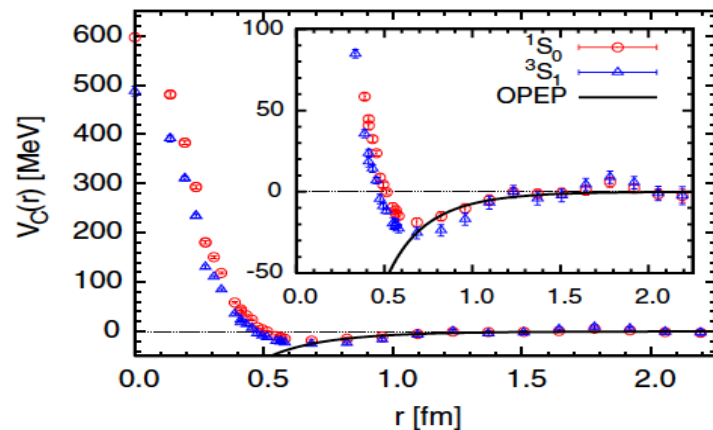


- particle physics, nuclear physics, astrophysics, ...

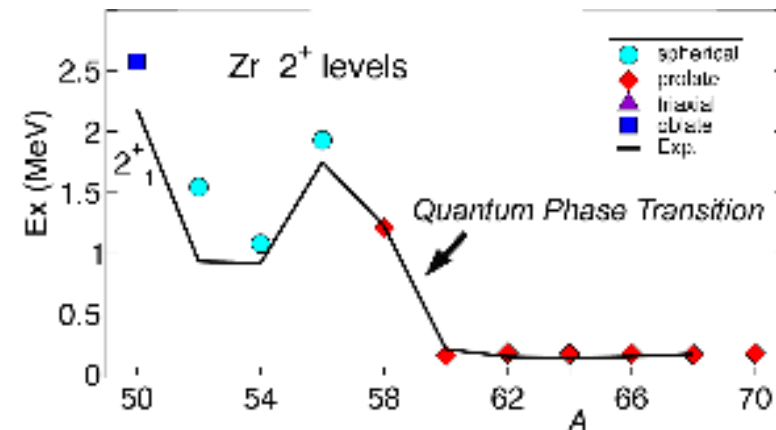
“K computer” launched in 2012
→ Post-K project in 2021



Hadrons : Lattice QCD
calculation to derive the potential



Nuclear structure : LSSM calc.
for exotic nuclei



Nuclear theory group in the University of Tokyo

Department of Physics

- Takaharu Otsuka
- Takashi Abe
- J. Menendez, T. Miyagi, S. Yoshida

Center for Nuclear Study

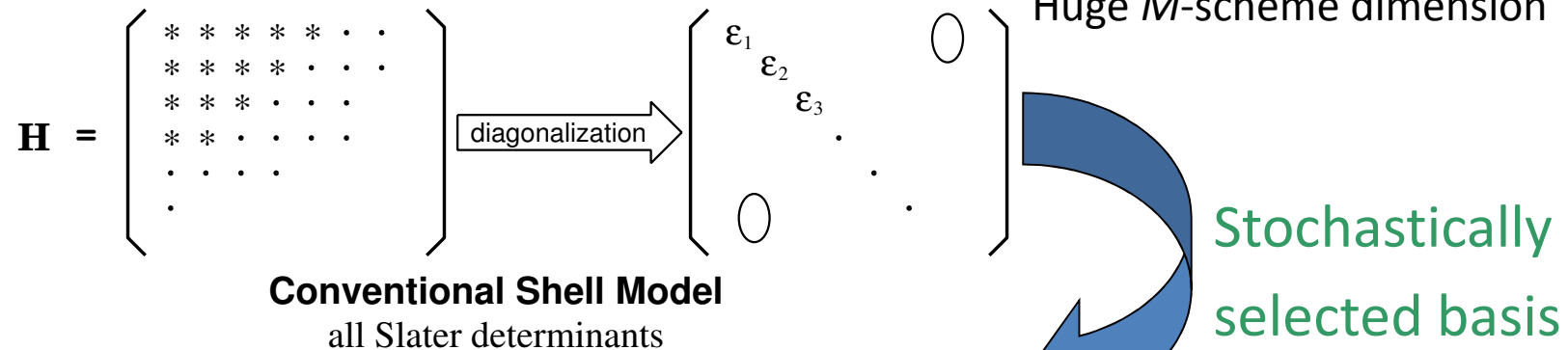
- Noritaka Shimizu
- T. Ichikawa, T. Togashi, N. Tsunoda, Y. Tsunoda, T. Yoshida
- Yutaka Utsuno (JAEA)

For no-core shell model calculations,
collab. with James Vary and Pieter Maris (Iowa State U)

Monte Carlo Shell Model

Otsuka, Honma, Mizusaki, Shimizu,
Utsuno, PPNP47, 319 (2001)

a tool to go beyond the conventional Lanczos diagonalization method
for Large-Scale Shell Model calculations



$$\mathbf{H} \approx \begin{pmatrix} * & * & * & \cdot \\ * & * & * & \cdot \\ * & * & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \xrightarrow{\text{diagonalization}} \begin{pmatrix} \epsilon'_1 & & 0 \\ & \epsilon'_2 & \\ 0 & & \cdot \end{pmatrix}$$

Monte Carlo Shell Model

bases important for a specific eigenstate

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

$\hat{h}(\sigma)$ one-body Hamiltonian

σ ... auxiliary fields

random numbers

$$|\Psi\rangle = \sum_{k=1}^{N_{MCSM}} f_k P^{J,\pi} |\phi_k\rangle \quad |\phi_k\rangle = \prod_{\alpha=1}^N \left(\sum_{i=1}^{N_{sp}} c_i^\dagger D_{i\alpha}^{(k)} \right) |-\rangle$$

↑ MCSM basis, deformed Slater det.

+ Further optimization + extrapolation with energy variance

= “advanced Monte Carlo shell model”

N. Shimizu *et al.*, PTEP 2012

MCSM wave function

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

$$|\Psi^{IM\pi}(N_b)\rangle = \sum_{d=1}^{N_b} f^{(d)} \sum_{K=-I}^I g_K^{(d)} \hat{P}^\pi \hat{P}_{MK}^I |\Phi(D^{(d)})\rangle$$

MCSM basis dimension ≈ 100

superposition

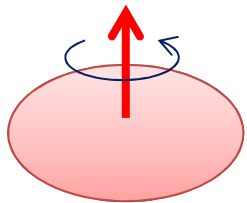
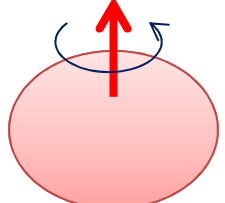
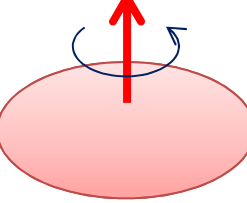
projection onto good
quantum numbers

optimized Slater
determinant

mixing with different shapes

rotation

deformed intrinsic state

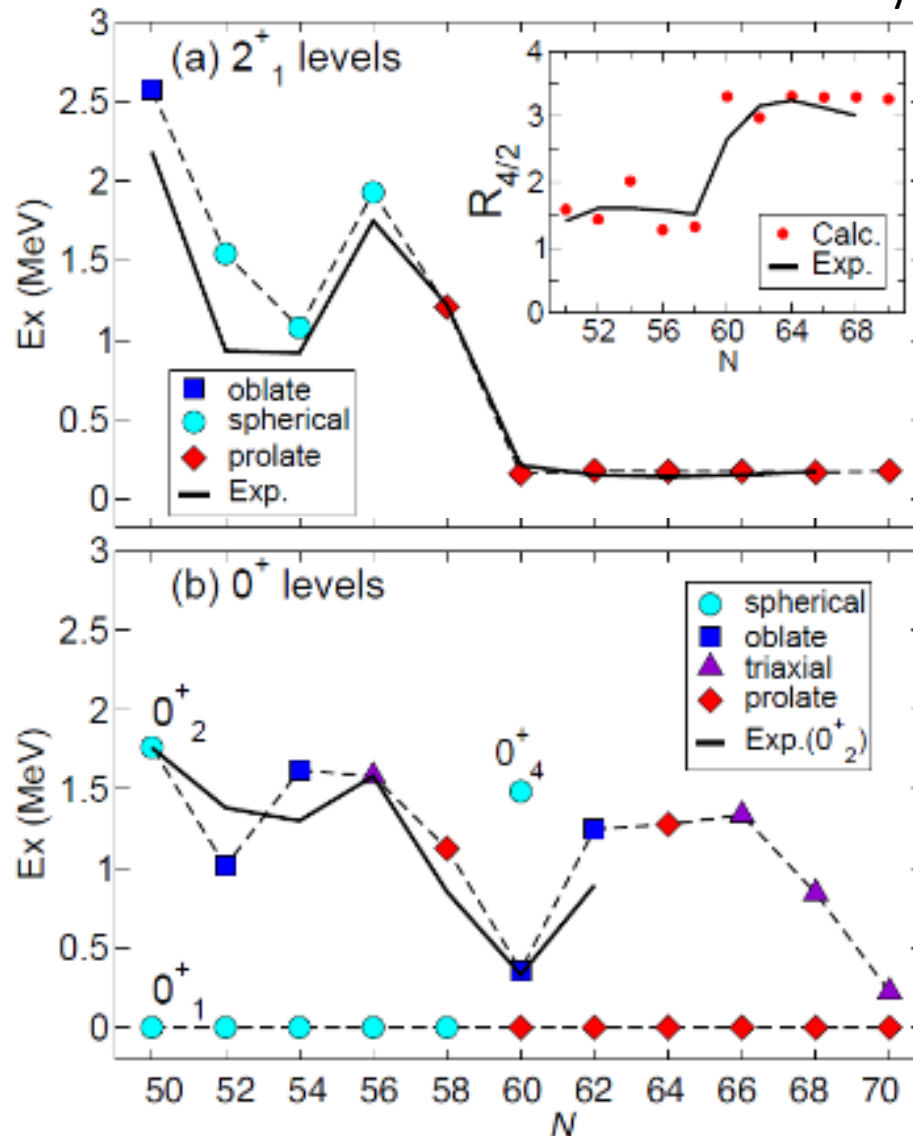
Wave function = $f^{(1)}$  + $f^{(2)}$  + $f^{(3)}$  +

$f^{(d)}, g_K^{(d)}, D^{(d)}$: variational parameters

MCSM enables us to discuss “intrinsic deformation”

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

T. Togashi, Y. Tsunoda, T. Otsuka and N. Shimizu,
Phys. Rev. Lett. accepted, arXiv:nucl-th 1606.09056



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

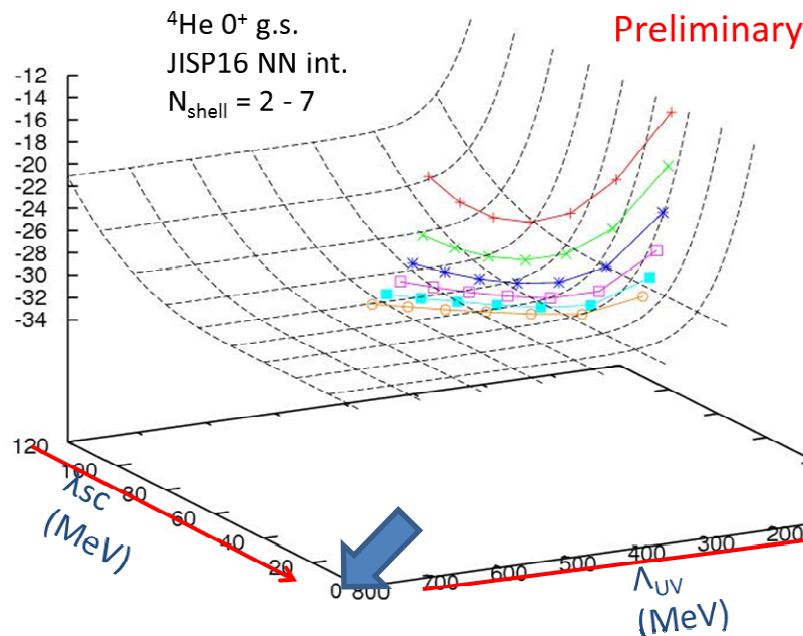
“quantum phase transition”
from spherical to prolate
deformation is shown by the
analysis of Monte Carlo shell
model (model space:
 $28 < Z < 70$, $40 < N < 94$, realistic
effective int.)

“Type-II shell evolution”
plays an important role.

T. Otsuka and Y. Tsunoda,
J. Phys. G 43, 024009 (2016)

No-core shell model calculations with MCSM + JISP16

T. Abe, P. Maris, T. Otsuka, N. Shimizu,
Y. Utsuno & J. P. Vary



Extrapolate energy eigenvalue to
infinitely large model space
using ultra-violet and infrared “cutoff”

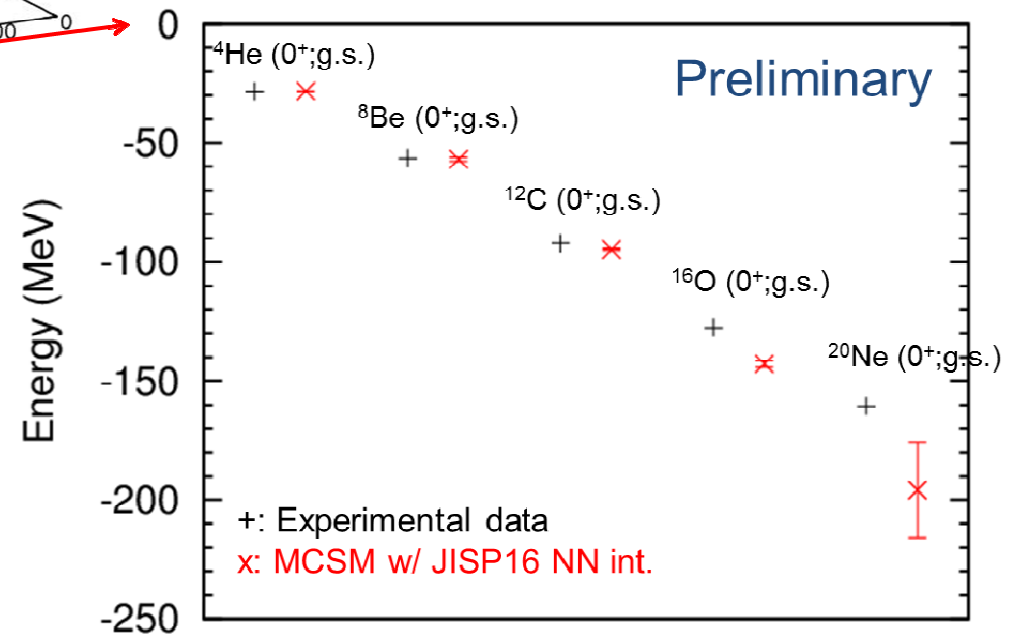
Infrared cutoff

$$\lambda_{sc} = \sqrt{m\hbar\omega/(N + 3/2)} - \lambda^2/\Lambda$$

Ultraviolet cutoff

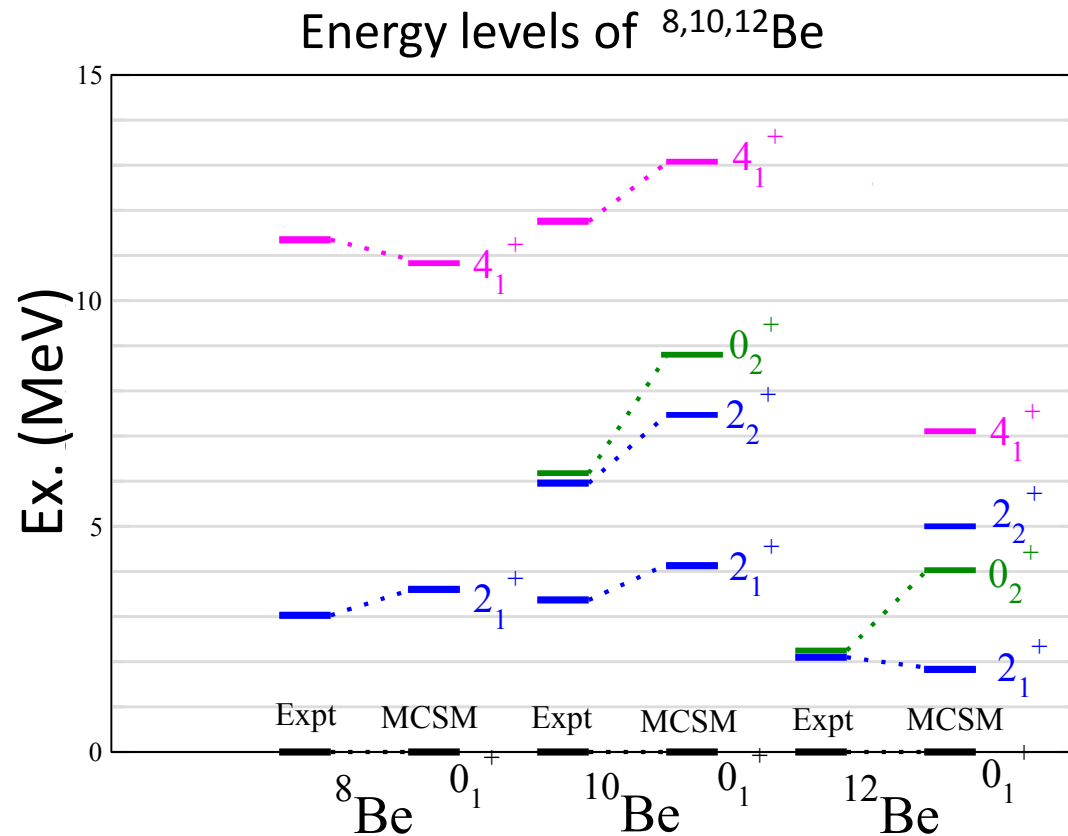
$$\Lambda = \sqrt{m(N + 3/2)\hbar\omega}$$

Binding energy of light nuclei:
up to 7 major shells as model space



no-core Monte Carlo shell model + JISP16

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



shell-model calculations
with $N_{shell} = 6$ and JISP16
interaction

overall tendency is good,
rather overestimated

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

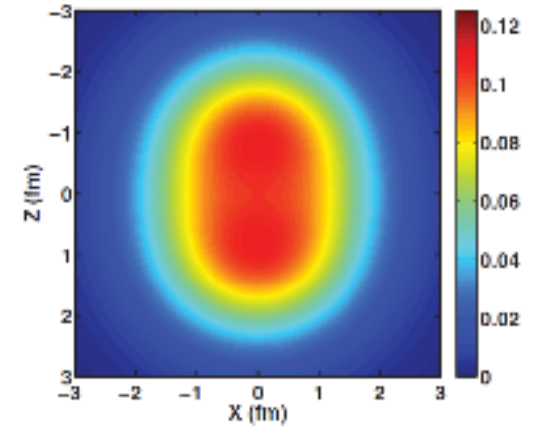
Intrinsic density in Monte Carlo shell model

cf. Translationally invariant density
 $^8\text{Li } 2+$ Cockrell *et al.*, PRC86 (2012)

Mean-field approx. + angular-momentum projection

$$|\Psi\rangle = P^J |\phi(D)\rangle$$

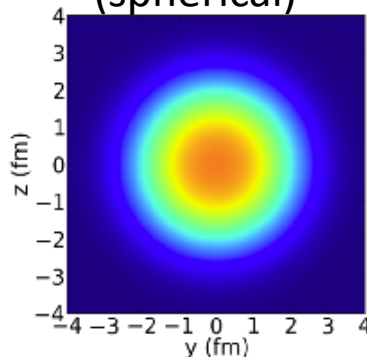
Slater determinant
 Intrinsic state



Monte Carlo shell model

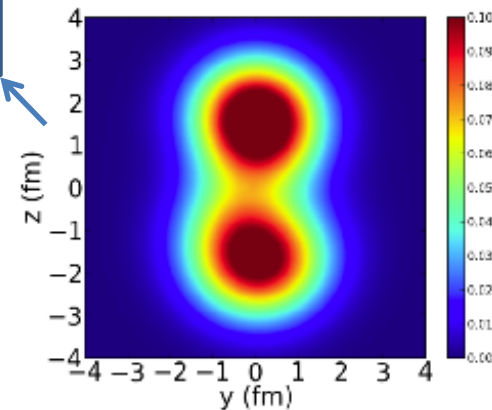
$$|\Psi\rangle = \sum_{k=1}^{N_{MCSM}} v_k P^{J,\pi} |\phi_k\rangle = P^{J,\pi} \left(\sum_{k=1}^{N_{MCSM}} v_k |\phi_k\rangle \right)$$

labo-system
 (spherical)



Angular-momentum
 projector

Intrinsic state



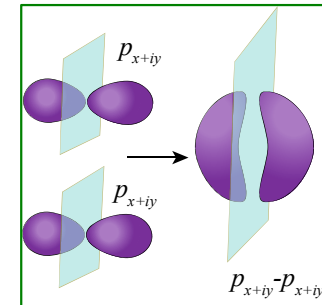
Density profile of ^8Be ground state

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

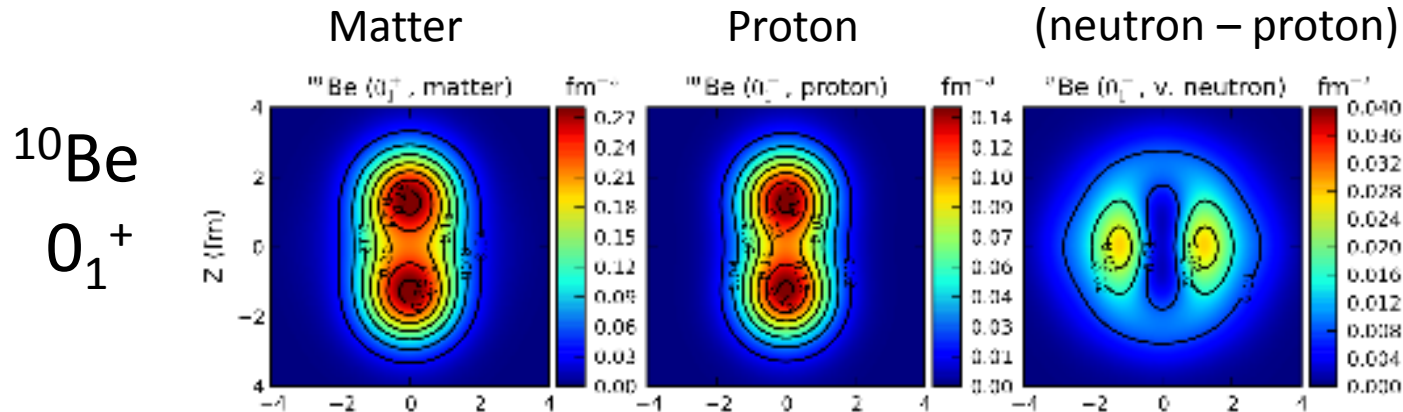
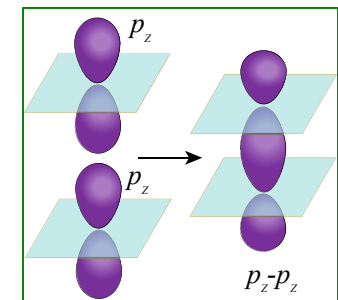
T. Yoshida, N. Shimizu, T Abe and T. Otsuka

Valence neutron
(neutron – proton)

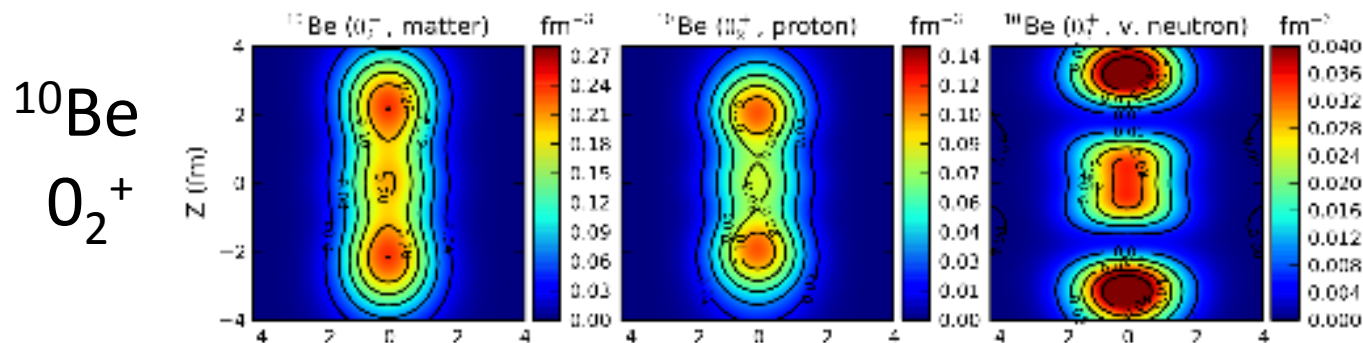
Pi molecular orbit



Sigma molecular orbit



Excited state



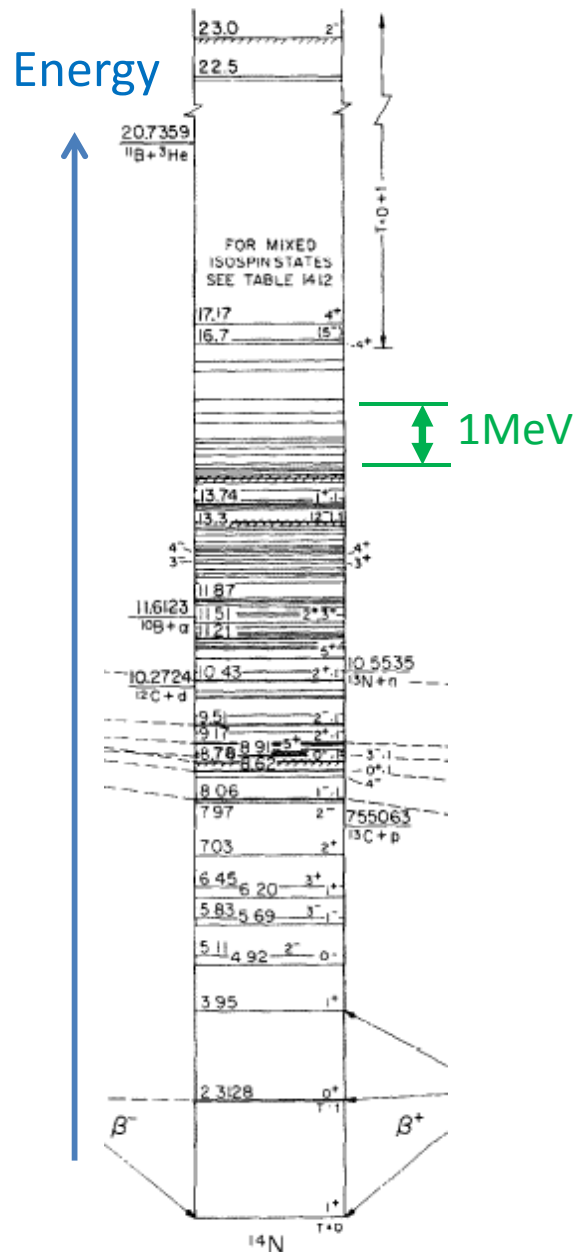
Elongation effect
for 2-alpha distance

Appearance of sigma
molecular orbit

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

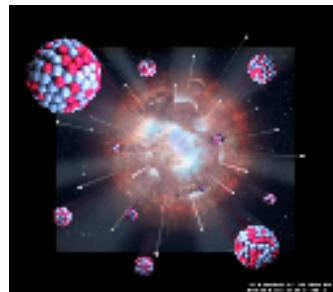
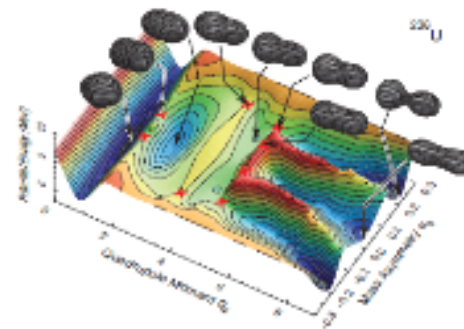
Noritaka Shimizu (U. Tokyo), Yutaka Utsuno (JAEA),
Yasunori Futamura (U. Tsukuba), Tetsuya Sakurai (U. Tsukuba),
Takahiro Mizusaki (U. Senshu), and Takaharu Otsuka (U. Tokyo)
Phys. Lett. B **753**, 13 (2016)

Nuclear level density

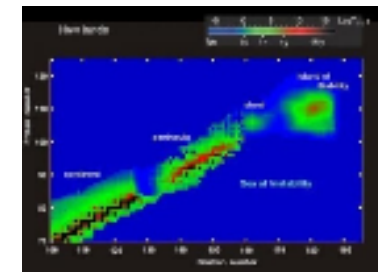


- Statistical model is important where the level density is large
- Hauser-Feshbach theory
 - input: Level density, γ -ray strength function, optical potential
 - output: neutron-capture cross section

Nuclear engineering



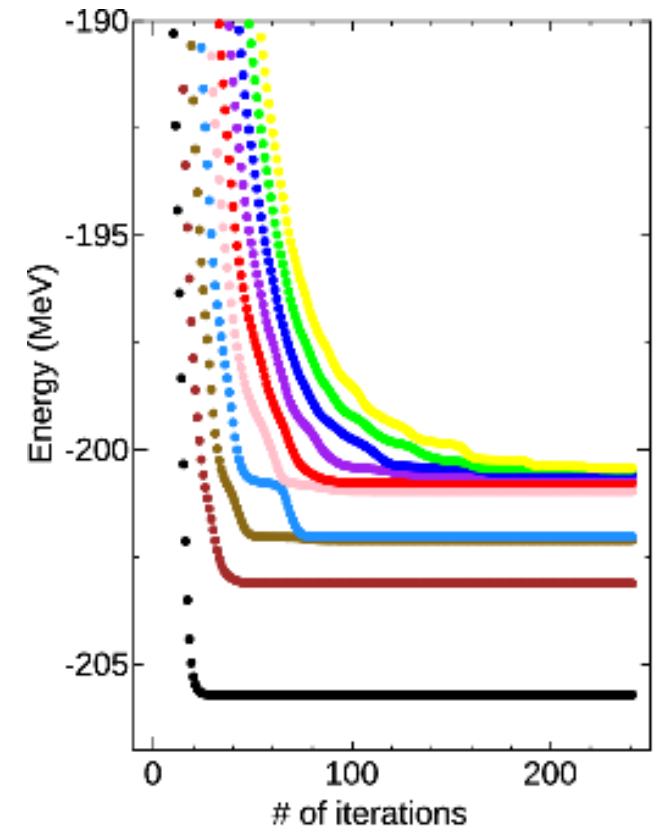
Nucleosynthesis



superheavy nuclei

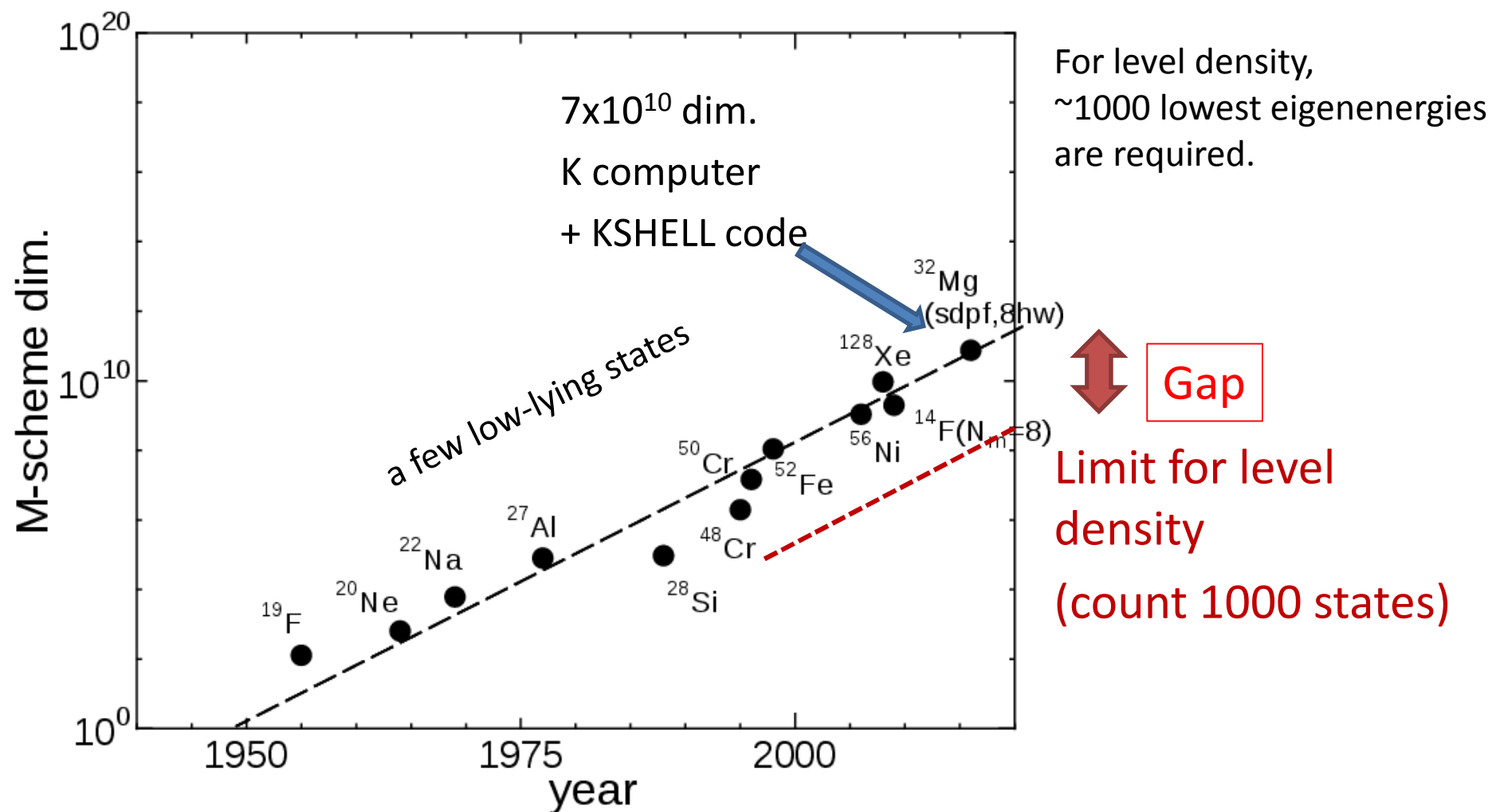
nuclear level density in LSSM

- 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

Current limitation of large-scale shell-model calc.



Level density in nuclear shell-model calc.

- Level density $\Rightarrow$ 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



Parallel stochastic estimation method of eigenvalue distribution

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odai, Tsukuba-shi, Ibaraki 305-8573, Japan

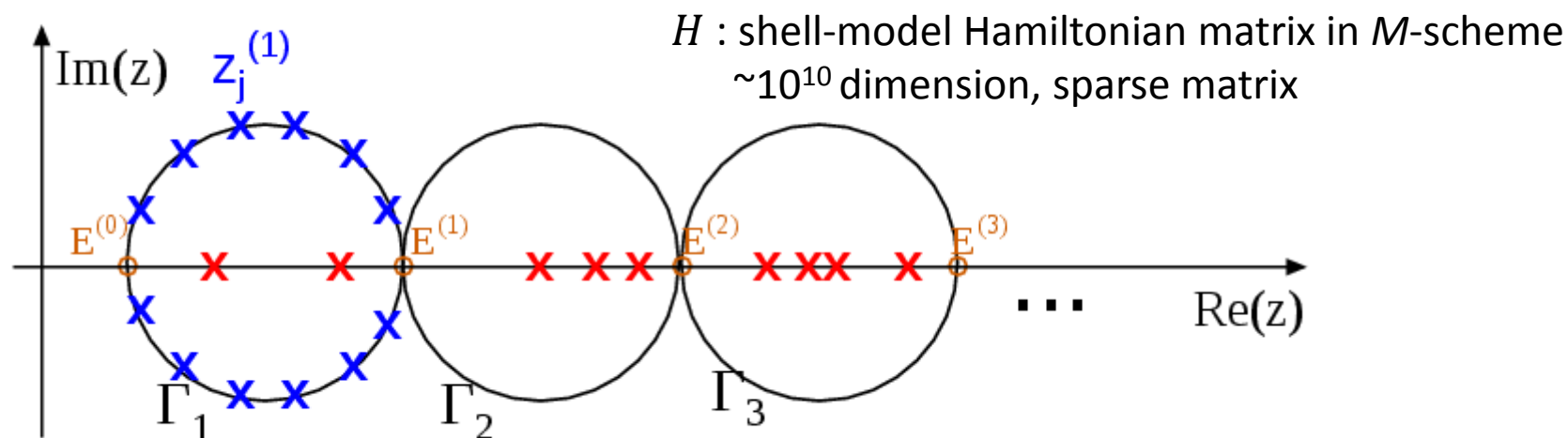
E-mail futamura@mma.cs.tsukuba.ac.jp

Received July 29, 2010, Accepted October 22, 2010



Counting eigenvalues : Cauchy integral

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



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

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

discretize

Next step : Stochastic estimation of trace

Hutchinson estimator

Estimate the matrix trace in Monte Carlo way

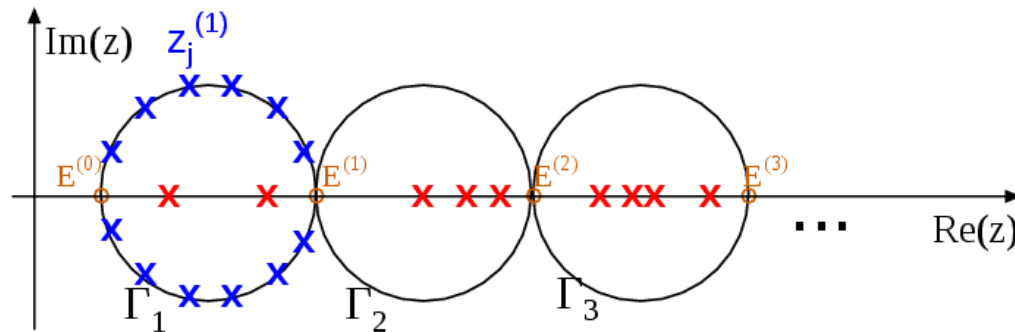
$$\text{Tr}(A) \cong \frac{1}{N_s} \sum_{i=1}^{N_s} v_i^T A v_i$$

- 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)
- $v_i^T A v_i = \text{Tr}(A) + \underbrace{\sum_{k \neq k'} (v_i)_k A_{kk'} (v_i)_{k'}}_{\text{Non-diagonal part}}$

Non-diagonal part

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

Stochastic estimation of “trace”



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

- estimating $\text{tr}(z - H)^{-1}$
 $= \sum_i^D \mathbf{e}_i^T (z - H)^{-1} \mathbf{e}_i$

D : Whole dimension

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

- Stochastic sampling

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

N_s : Number of samples

$N_s=32$ show Next step : Matrix inverse

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

→ solve linear equations to avoid the inverse of matrix

$$\begin{aligned} \text{solve } \mathbf{v}_i &= (z - H) \mathbf{x}_i & \text{and obtain } \mathbf{v}_i^T \mathbf{x}_i \\ \mathbf{v}_i &= A \mathbf{x}_i \end{aligned}$$

Complex Orthogonal Conjugate Gradient (COCG)

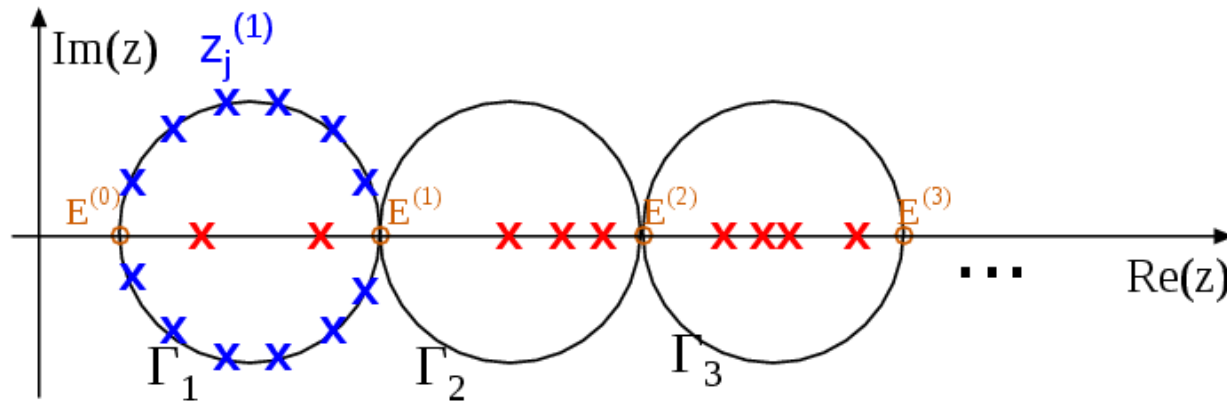
$$\begin{aligned} x_{k+1} &= x_k + \alpha_k p_k, & \alpha_k &= r_k^T r_k / p_k^T A p_k \\ r_{k+1} &= r_k - \alpha_k \boxed{A p_k}, & \beta_k &= r_{k+1}^T r_{k+1} / r_k^T r_k \\ p_{k+1} &= r_{k+1} + \beta_k p_k, \end{aligned}$$

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 ...

⇒ Shift algorithm

solve $\mathbf{v}_i = (z_{ref} - \sigma - H) \mathbf{x}_i$ σ : shift
using solution of solve $\mathbf{v}_i = (z_{ref} - H) \mathbf{x}_i$

Shift invariance of Krylov subspace

- Purpose : solve $A\mathbf{x} = \mathbf{b}$ and $(A - \sigma)\mathbf{x} = \mathbf{b}$ 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 $A\mathbf{x} = b$ is always on the Krylov subspace
- Is the solution of $(A - \sigma)\mathbf{x} = b$?

$\Rightarrow$ It is on the same Krylov subspace

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

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

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

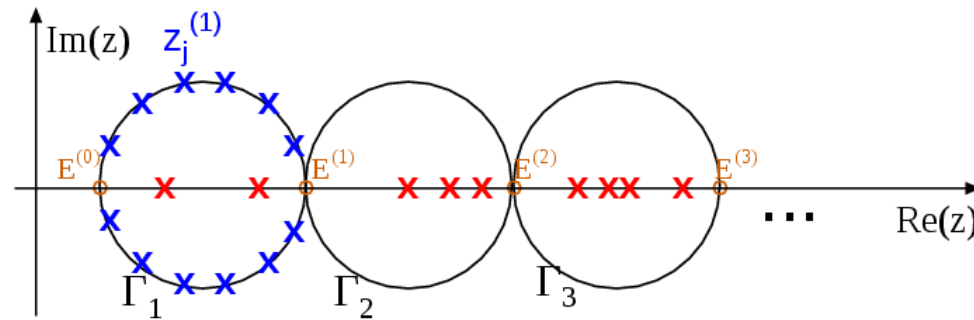
$$\pi_{k+1}^\sigma = (1 + \alpha_k \sigma) \pi_k^\sigma + \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}} (\pi_k^\sigma - \pi_{k-1}^\sigma),$$

$$\alpha_k^\sigma = \frac{\pi_k^\sigma}{\pi_{k+1}^\sigma} \alpha_k,$$

$$\beta_k^\sigma = \left(\frac{\pi_k^\sigma}{\pi_{k+1}^\sigma} \right) \beta_k$$

Recipe for estimating level density

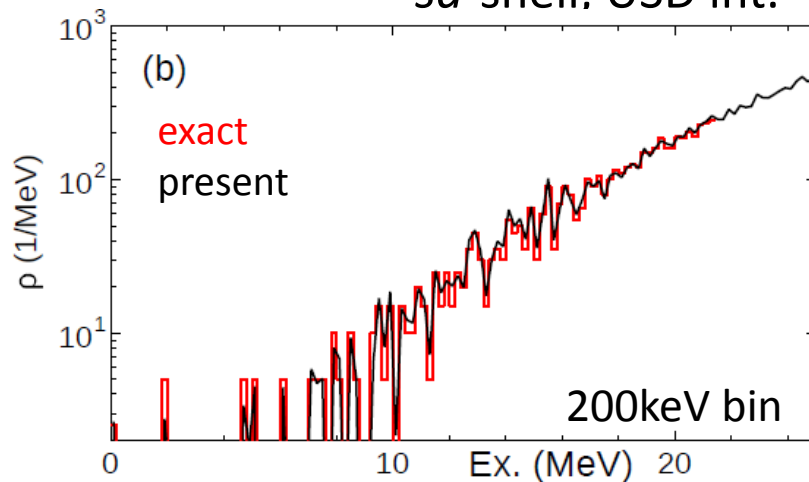
$$\mu_k = \frac{1}{2\pi i} \oint_{\Gamma_k} dz \operatorname{tr}((z - H)^{-1})$$



- Prepare mesh points $z_j^{(k)}$ to calculate the contour integral of z .
- Prepare random vectors $\mathbf{v}_i$ to estimate trace with Hutchinson estimator.
- Solve $(z - H)\mathbf{x}_i = \mathbf{v}_i$ by Block COCG method to obtain $\mathbf{v}_i^T (z - H)^{-1} \mathbf{v}_i$
- $\mathbf{v}_i^T \left(z_j^{(k)} - H \right)^{-1} \mathbf{v}_i$ for any j, k are calculated by shift algorithm

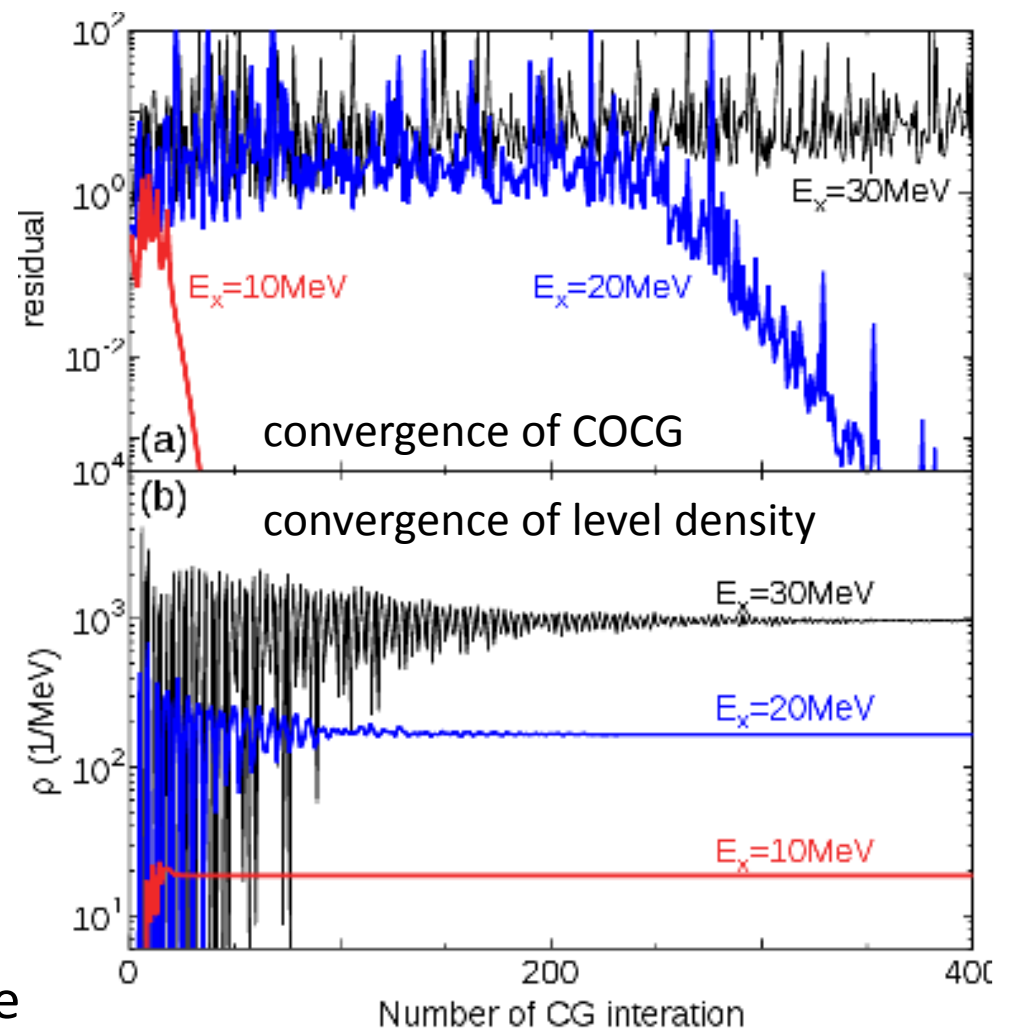
Benchmark test

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

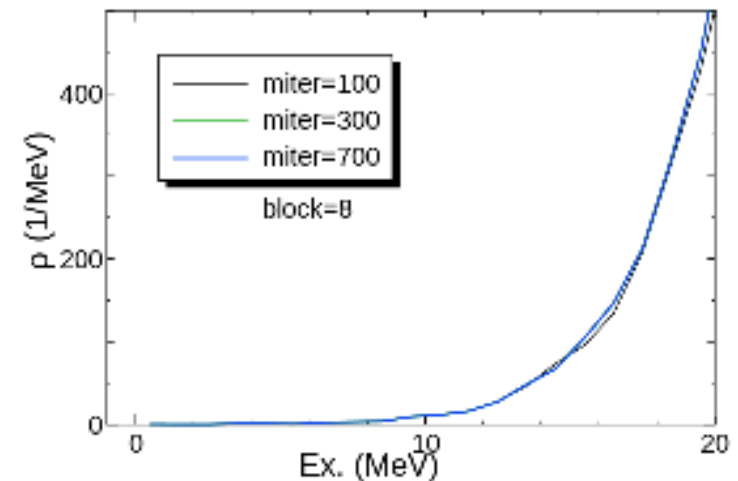
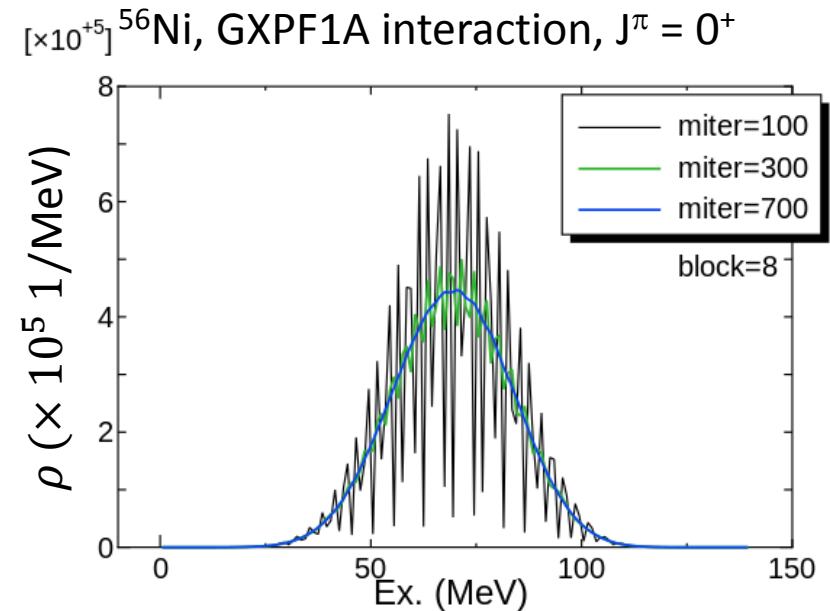


Benchmark of spin-dependent level density at large-scale problem

- Spin-dependent level density: replace initial sample vectors of M -scheme, $\mathbf{v}_i$, by angular-momentum projected vectors $P^J \mathbf{v}_i$

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

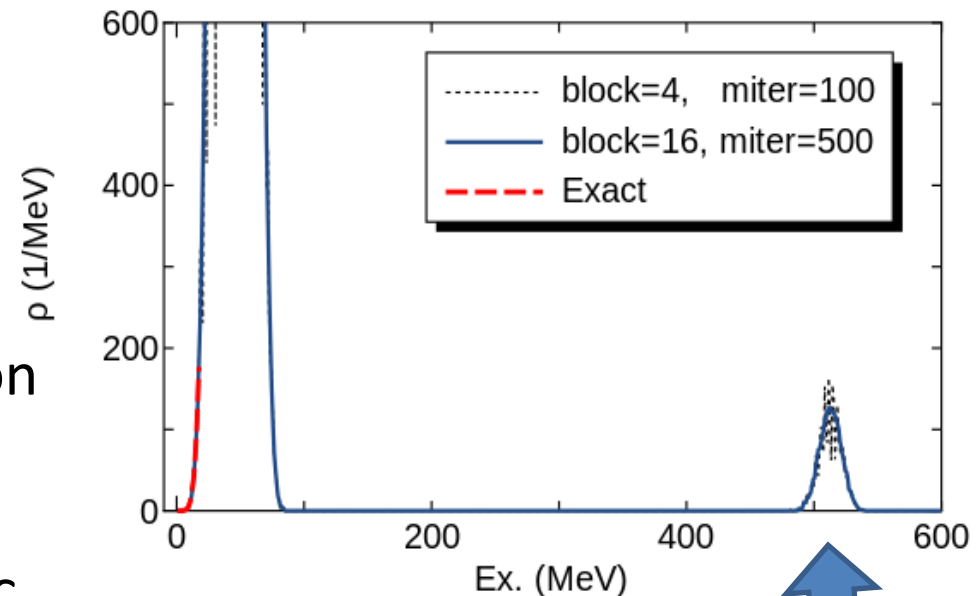
- ^{56}Ni in pf-shell
 1.0×10^9 M -scheme dimension,
 1.5×10^7 J -scheme dimension
 impossible to obtain level density by conventional Lanczos method
- To converge the level density in whole energy region, 700 COCG iterations are required.
- 100 COCG iterations are enough for low-energy region



Subtract spurious center-of-mass states (Lawson method)

$$H' = H + \beta_{\text{CM}} H_{\text{CM}}$$

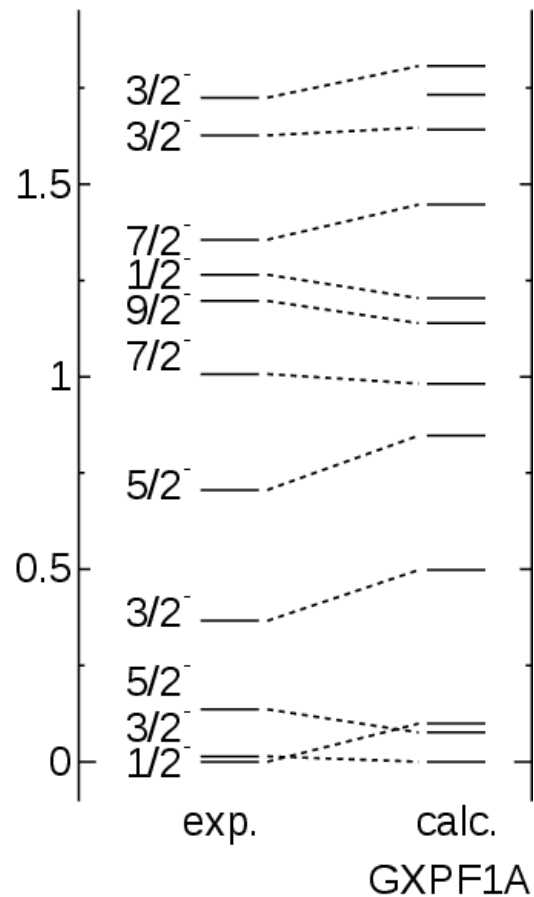
- ^{48}Ca $J=1^-$, sd - pf - sdg shell, $1\hbar\omega$ truncation
- Lift up spurious center-of-mass excited states by Lawson method clearly.
- agree well with the exact calc.



Spurious state by center-of-mass excitation

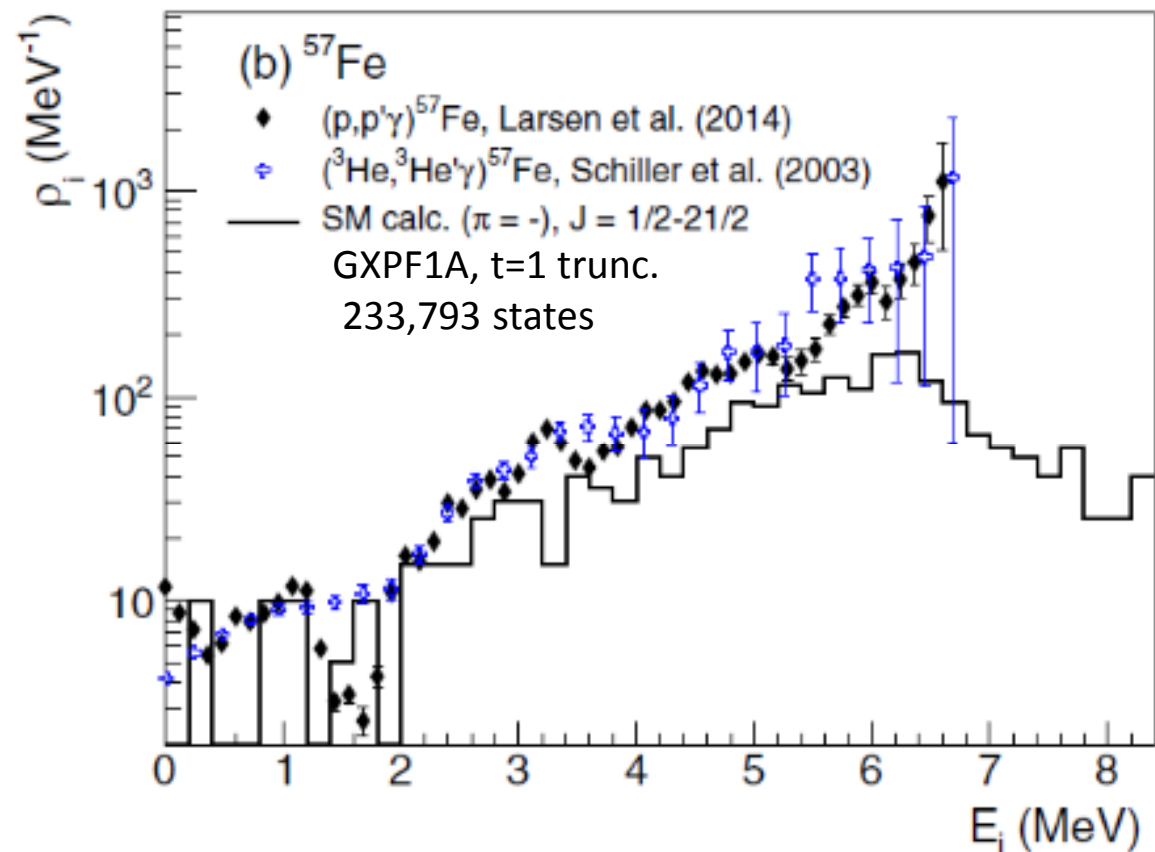
comparison with experiment: level density of ^{57}Fe

low-lying levels



Level density

exp. vs SM Lanczos method



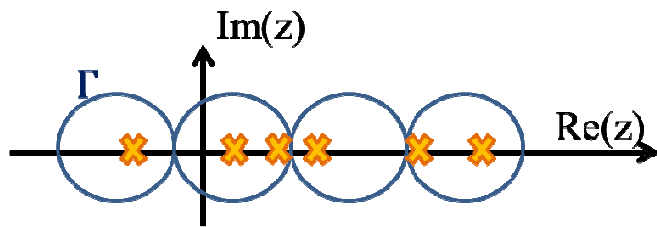
B. A. Brown and A. C. Larsen, PRL 113, 252502 (2014)

Realistic interaction gives a unified description of low-lying spectroscopy and level density in low-energy region

Level density by large-scale shell model calc.

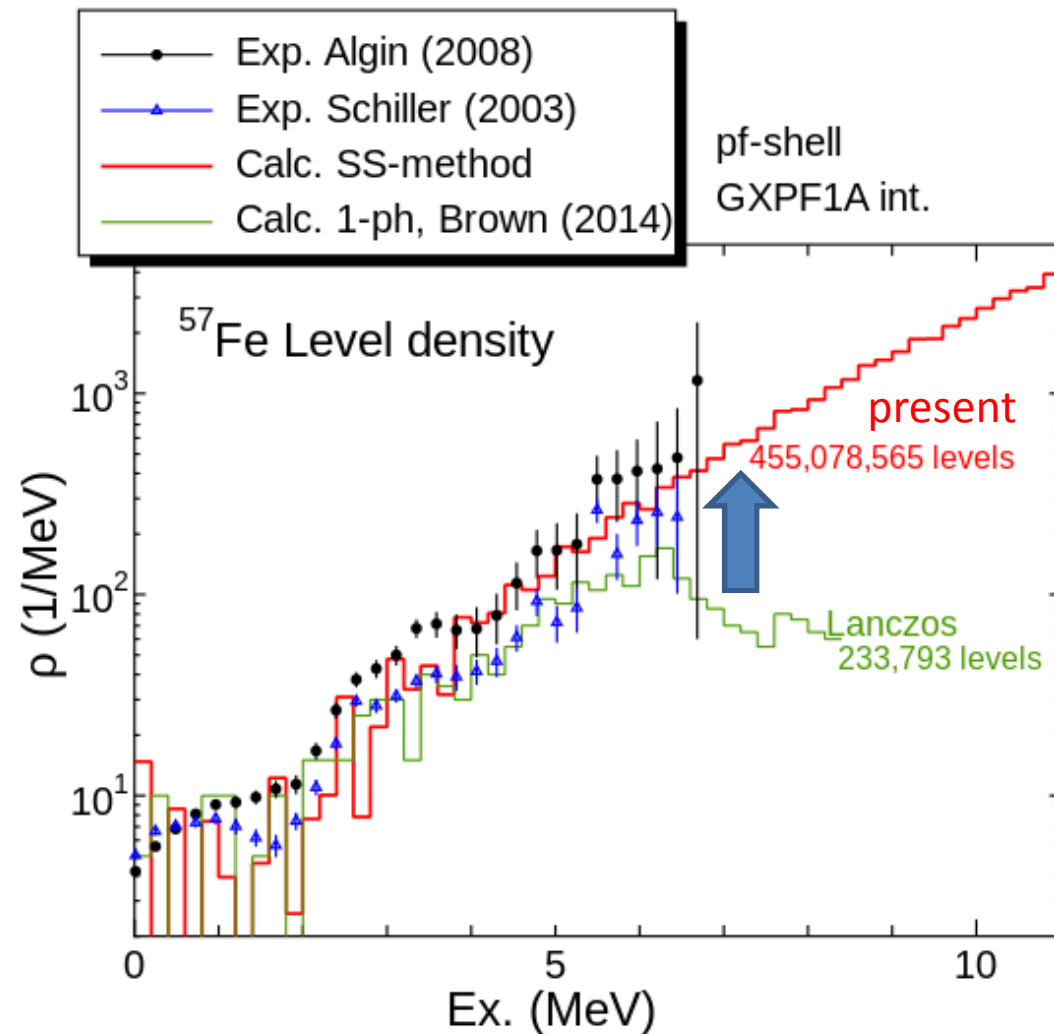
Stochastic estimation for density of states

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



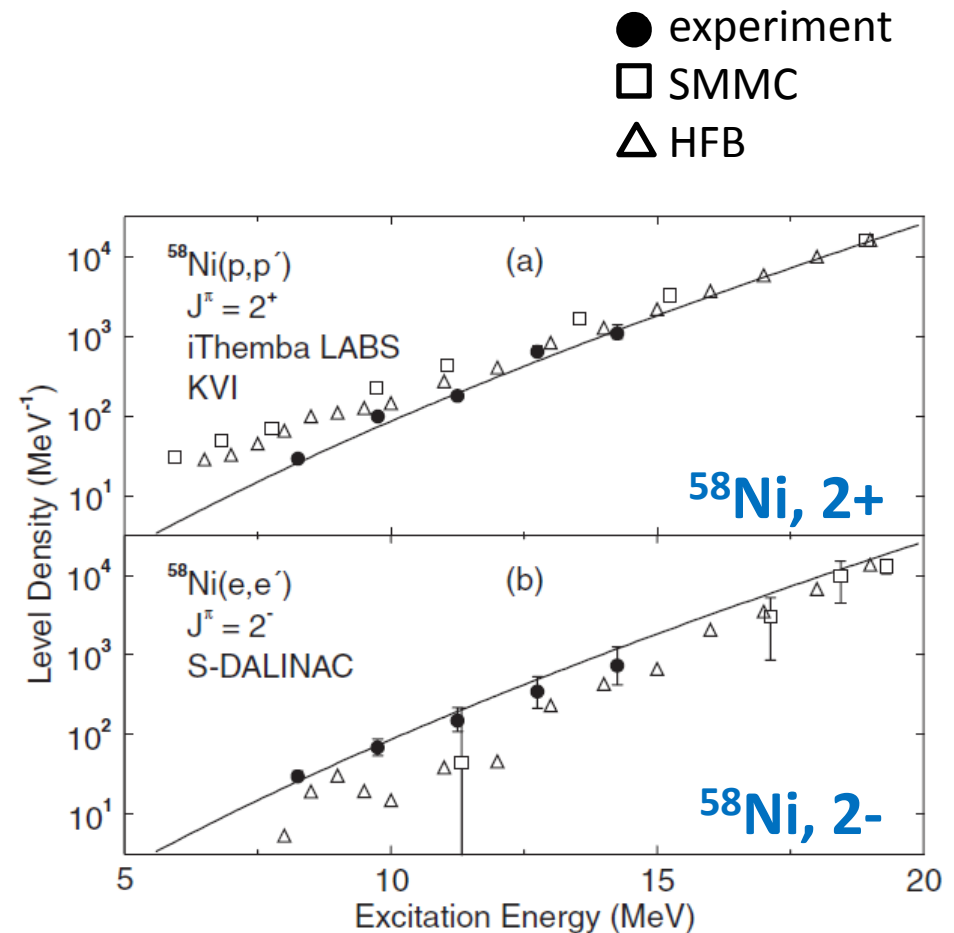
$$\begin{aligned} \rho(E) &\approx \frac{1}{N} \sum_i \oint_{\Gamma} \vec{v}_i (z-H)^{-1} \vec{v}_i dz \\ &\approx \frac{1}{N} \sum_{i,j} w_j \vec{v}_i (z_j-H)^{-1} \vec{v}_i \end{aligned}$$

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



Puzzle: parity dependence of level density

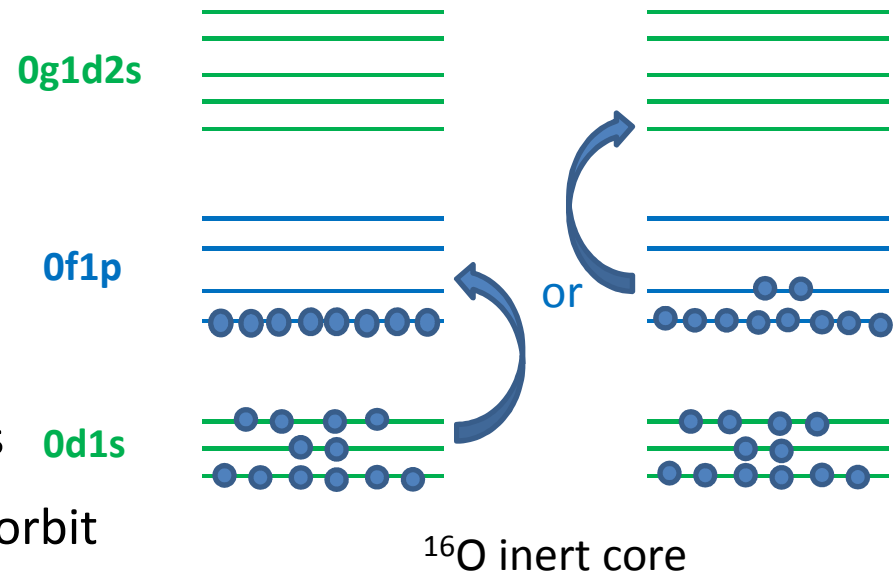
- Spin-parity dependence:
crucial for application (due to selectivity)
- Parity-equilibration of level density is often assumed by empirical formulas
- Experiment shows that $2+$ and $2-$ level densities of ^{58}Ni are similar value to each other (Kalmykov 2007)
- Microscopic calculations (SMMC, HFB-based 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

Nucl.	J^π	E_x (MeV)		j	C^2S	
		Cal.	Exp.		Cal.	Exp.
^{57}Co	$7/2_1^-$	0	0	$\pi 0f_{7/2}^{-1}$	5.28	4.27, 5.53
$^{58}\text{Ni} - p$	$1/2_1^+$	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
$^{58}\text{Ni} - n$	$1/2_1^+$	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
$^{58}\text{Ni} + p$	$9/2_1^+$	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
$^{58}\text{Ni} + n$	$9/2_1^+$	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

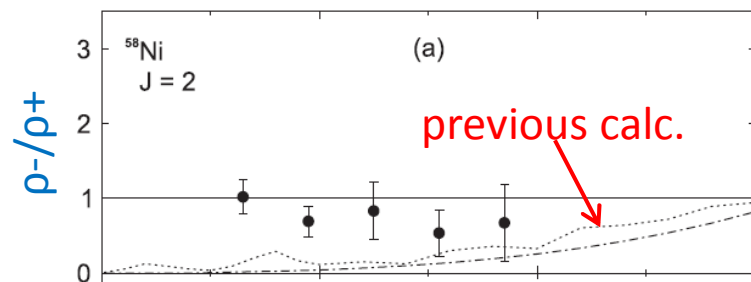
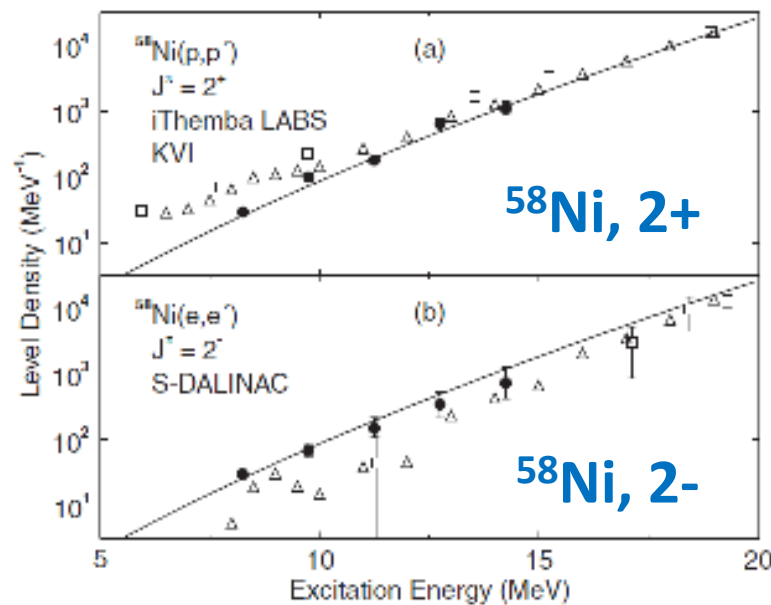
SDPF-MU int. Y. Utsuno *et al.*, PRC 86, 051301R (2012)
 VMU int. T. Otsuka *et al.*, PRL 104, 012501 (2010)

Single-particle characters of $^{58}\text{Ni} \pm p, n$
 are successfully described by LSSM

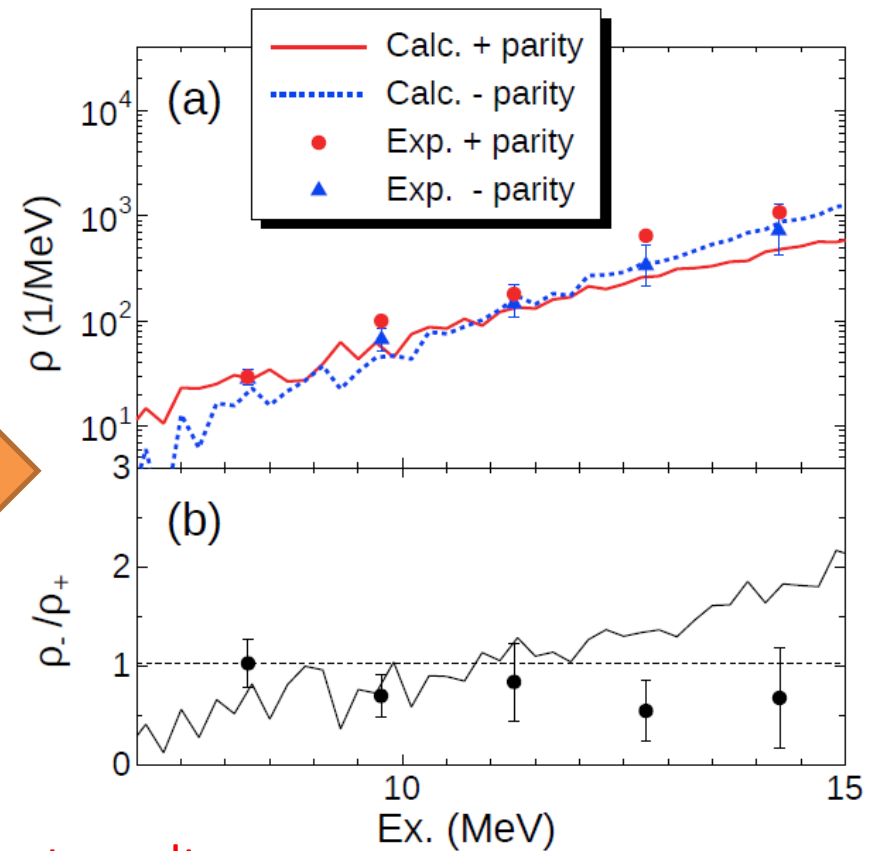
Application: parity dependence of level density

Contradiction between experiment and theory is resolved.

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



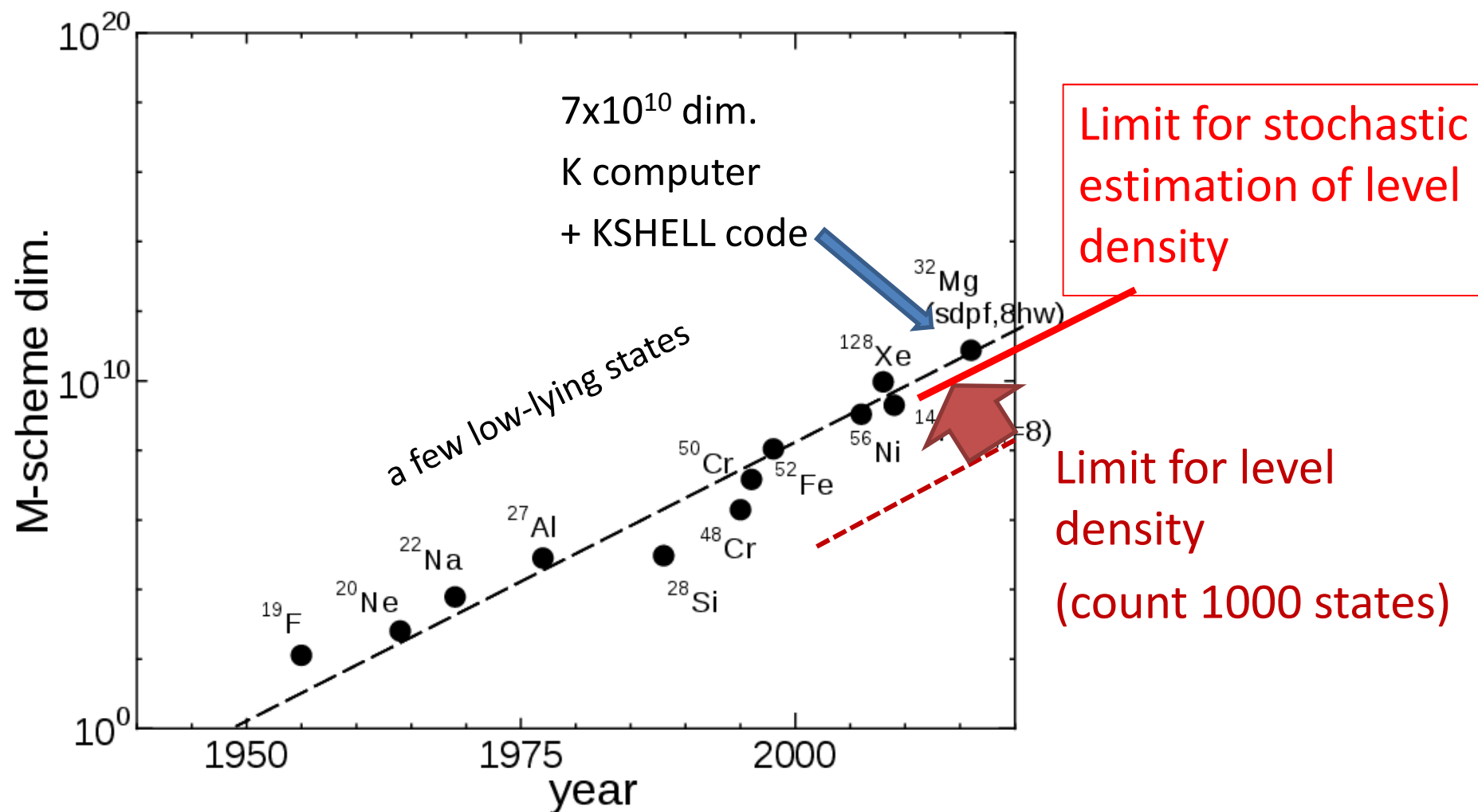
Ref. Y. Kalmykov *et al.*, PRL **99**, 202502 (2007).



Present result

Common setup to the study of exotic nuclei

Current limitation of large-scale shell-model calc.



Summary of LSSM level-density study

- We introduced a new stochastic estimation of level density in nuclear shell-model calculations utilizing conjugate gradient method.
 - Features: possible to treat any realistic interaction, spin-parity dependence, and removal of center-of-mass contamination.
 - Computational cost: similar order to obtaining a few low-lying states in Lanczos method
 - Benchmark : level densities by the new method agree well with the exact Lanczos results. Good convergence is seen.
- 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