核力から出発した非現象論的な中重原子核構造の研究~多体摂動論と大規模殻模型計算を用いて

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2017/02/16, 「京からポスト京に向けて」シンポジウム

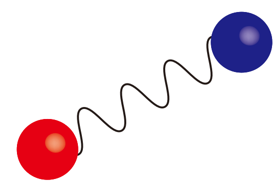
N.T., K. Takayanagi, M. Hjorth-Jensen, and T. Otsuka, Phys. Rev. C **89**, 024313 (2014).
N.T., T. Otsuka, N. Shimizu, M. Hjorth-Jensen, K. Takayanagi, T. Suzuki, Phys. Rev. C. Rapid. accepted.

- Introduction
- Construction of Effective interaction
- Application to island of inversion (京でやったこと)
- Application to pf+sdg-shell nuclei (ポスト京に向けて)
- Conclusion

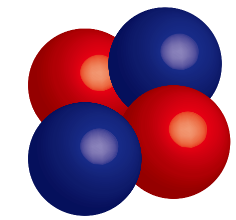
Construction of “Bridges”

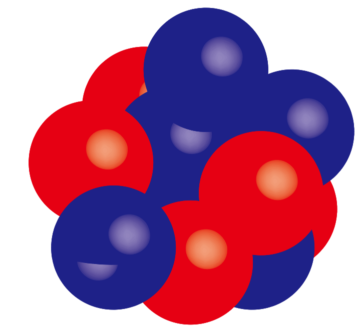
QCD

Nuclear force



Light nuclei ~A≒10-20



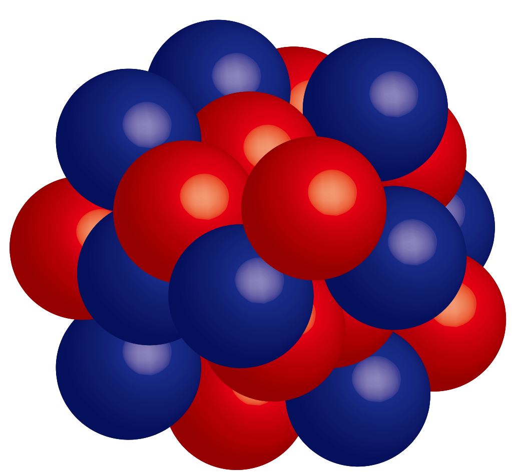


Lattice QCD
Effective Field Theory

Few body techniques
No core shell model
and many others…

This work

Medium mass nuclei~A≒20-100

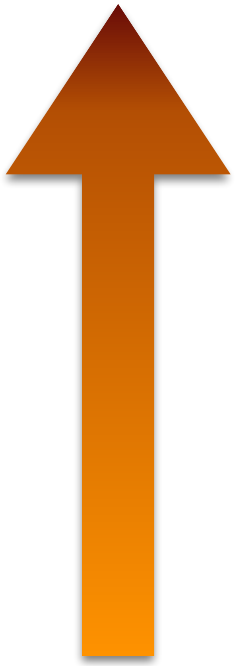


shell model with core
via the **effective interaction**
derived from **nuclear force**

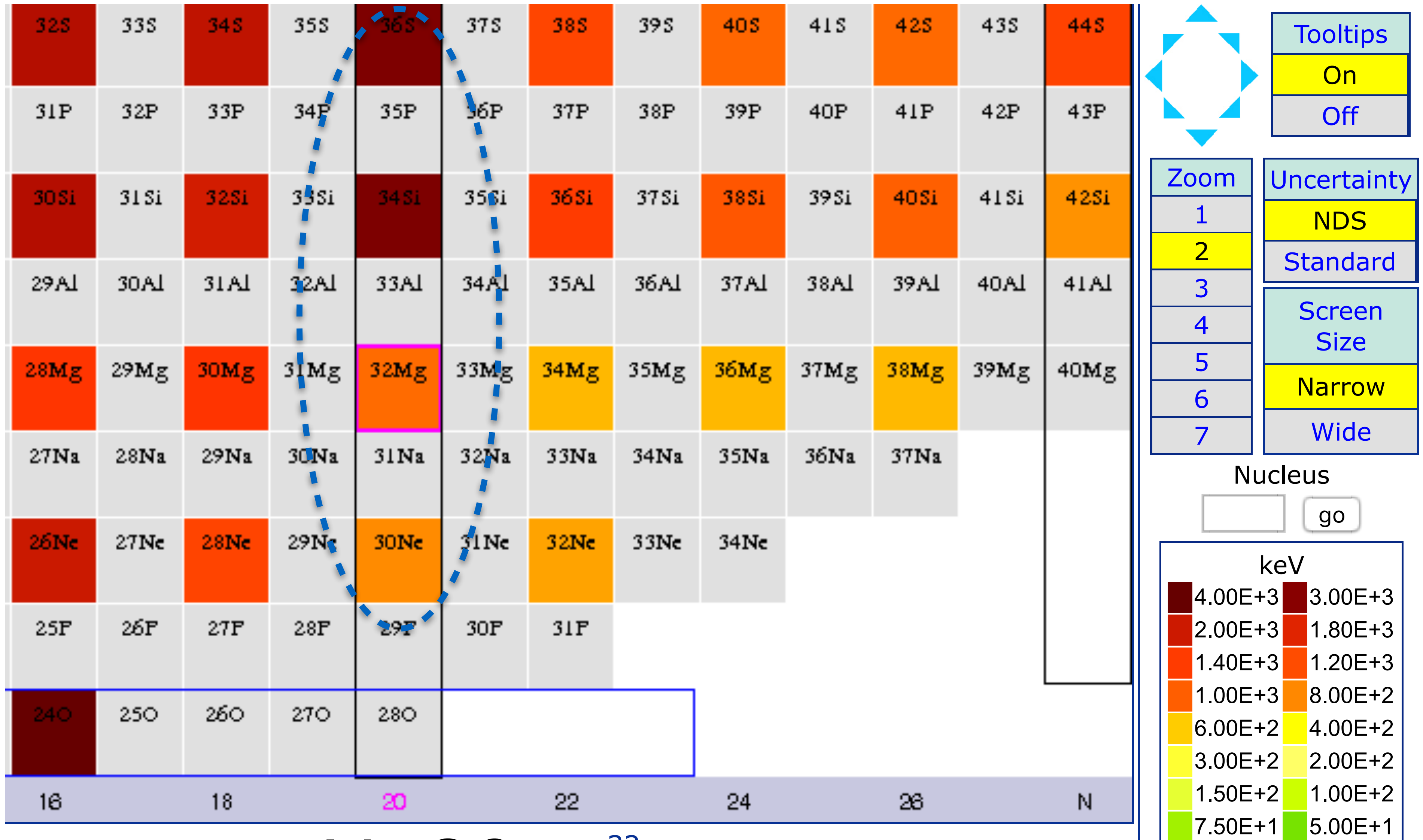
Neutron-rich nuclei~ island of inversion

http://www.nndc.bnl.gov/nudat2/reCenter.jsp?z=12&n=20

shell gap



breaking of shell gap



N=20

- E(2+)~1 MeV on N=20 indicate **breaking** of major shell gap
- Unified treatment of beyond and below the N=20 gap is necessary
- And this is one of many examples….

Nuclear force and Nuclear shell model

Single particle energies

Shell model Hamiltonian $$H = \sum_i \epsilon_i a_i^\dagger a_i + \sum_{ijkl} V_{ij,kl} a_i^\dagger a_j^\dagger a_l a_k.$$

two-body matrix elemetns

i, j, k, l : relevant degrees of freedom = **model space**

What we aim at is to:

- **derive** Shell model Hamiltonian based on **Nuclear force**
- **diagonalize this Hamiltonian** to know nuclear properties

What we need is:

- **Many-body theory** to derive Hamiltonian for **desired** model space
  - neutron-rich nuclei need large model space
- **Large scale shell model calculation (Large scale Lanczos diagonalization and Monte Calro Shell model)**

- Introduction
- **Theory of Effective interaction**
- Application to island of inversion (京でやったこと)
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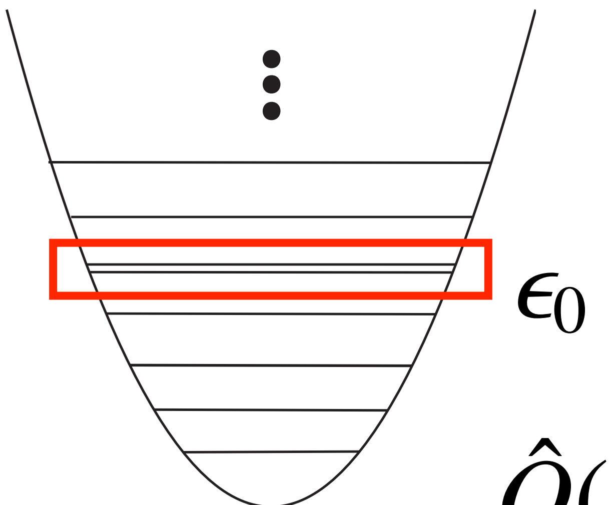
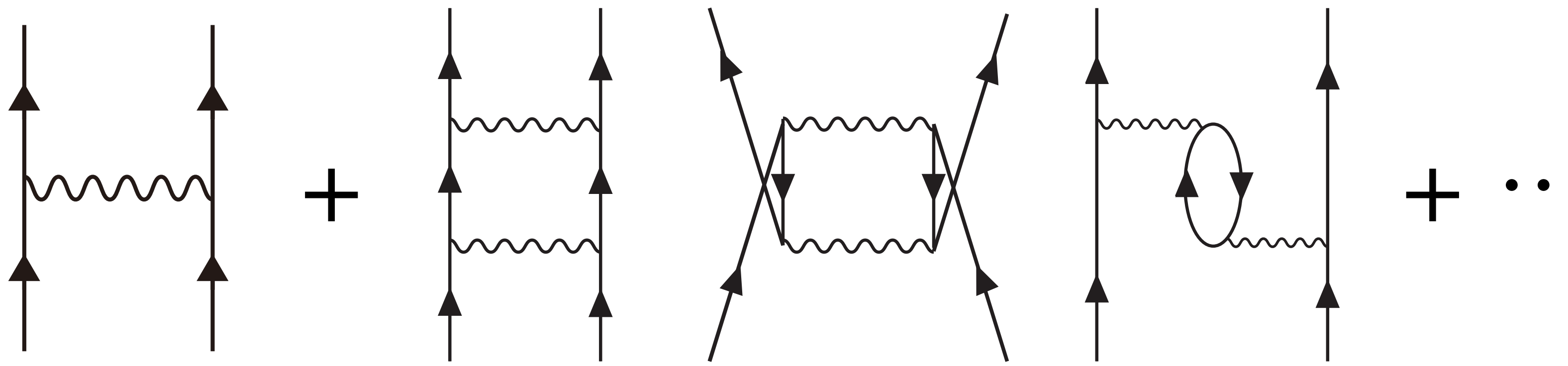
Many-body perturbation theory

P: model space

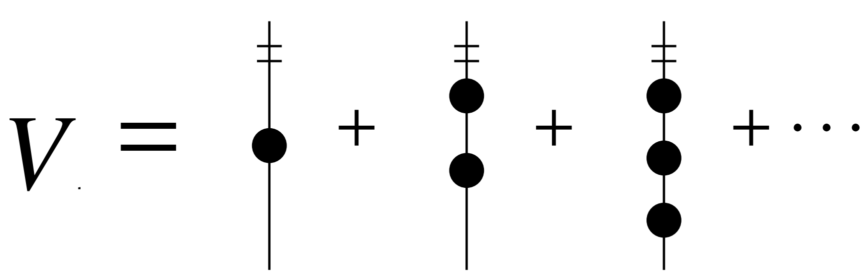




$$\hat{Q}(E) = PVP + PVQ\frac{1}{E - QHQ}QVP$$

Q-box

As non-perturbative correction, we further include infinite repetition of Q-box



some algebra···

non-perturbative correction

$$V_{\rm eff}^{(n)} = \hat{Q}(\epsilon_0) + \sum_{k=1}^{\infty} \hat{Q}_k(\epsilon_0)\{V_{\rm eff}^{(n-1)}\}^k.$$

$$\hat{Q}_k(E) = \frac{1}{k!}\frac{{\rm d}^k \hat{Q}(E)}{{\rm d}E^k}.$$

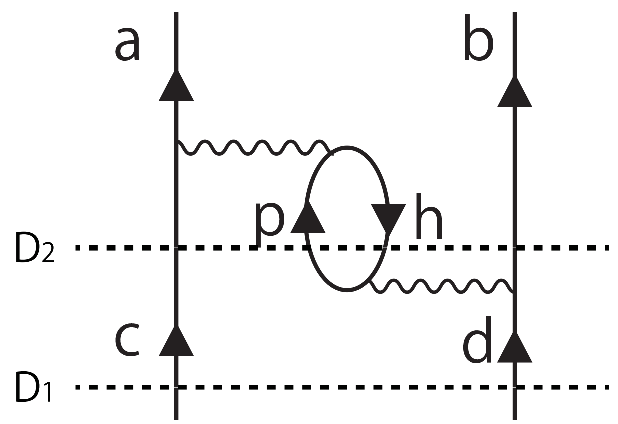
:Q-box

Divergent problem of Q-box in non-degenerate model space

(A)KK method requires assumption that the model space is **degenerate**

(B)Naive perturbation theory leads a **divergence** in non-degenerate model space

Example



$$\frac{V_{ah,cp}V_{pb,hd}}{(\epsilon_c+\epsilon_d)-\epsilon_c-\epsilon_p+\epsilon_h-\epsilon_b}$$

⟶ **Energy denominator is zero when $\varepsilon_d - \varepsilon_b = \varepsilon_p - \varepsilon_h$**

We need a theory which satisfies

(a)The assumption of degenerate model space is **removed**

(b)**Avoid** the divergence appearing in Q-box diagrams

→ **EKK method as a re-summation scheme of KK method**

Extended KK method as a re-summation of the perturbative series

EKK method

New parameter E (arbitrary parameter)

$$\begin{aligned} H &= H_0' + V' \\ &= \begin{pmatrix} E & 0 \\ 0 & QH_0Q \end{pmatrix} + \begin{pmatrix} P\tilde{H}P & PVQ \\ QVP & QVQ \end{pmatrix}, \end{aligned}$$

$$H_{\rm BH}(E) = PHP + PVQ\frac{1}{E - QHQ}QVP.$$

$$\tilde{H}_{\rm eff}^{(n)} = \tilde{H}_{\rm BH}(E) + \sum_{k=1}^{\infty} \hat{Q}_k(E)\{\tilde{H}_{\rm eff}^{(n-1)}\}^k$$

KK method (conventional)

$$\begin{aligned} H &= H_0 + V \\ &= \begin{pmatrix} PH_0P & 0 \\ 0 & QH_0Q \end{pmatrix} + \begin{pmatrix} PVP & PVQ \\ QVP & QVQ \end{pmatrix} \end{aligned}$$

$$\hat{Q}(E) = PVP + PVQ\frac{1}{E - QHQ}QVP$$

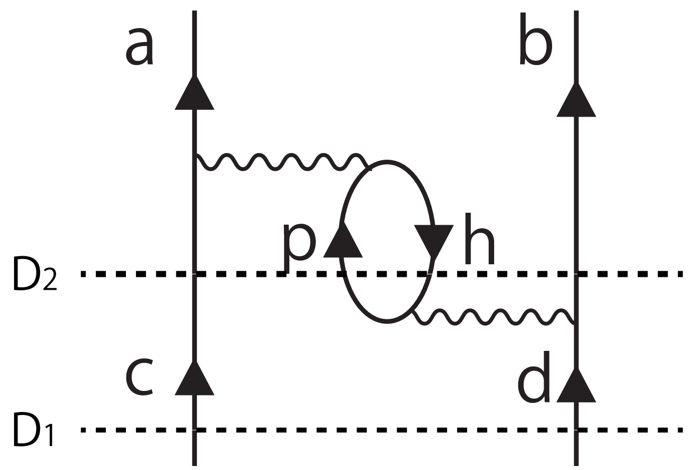
$$V_{\rm eff}^{(n)} = \hat{Q}(\epsilon_0) + \sum_{k=1}^{\infty} \hat{Q}_k(\epsilon_0)\{V_{\rm eff}^{(n-1)}\}^k.$$

- EKK method can be interpreted as a re-summation of KK method
- All the arguments are kept unchanged with the new division of the Hamiltonian

N. Tsunoda, K. Takayanagi, M. Hjorth-Jensen, and T. Otsuka, Phys. Rev. C 89, 024313 (2014).

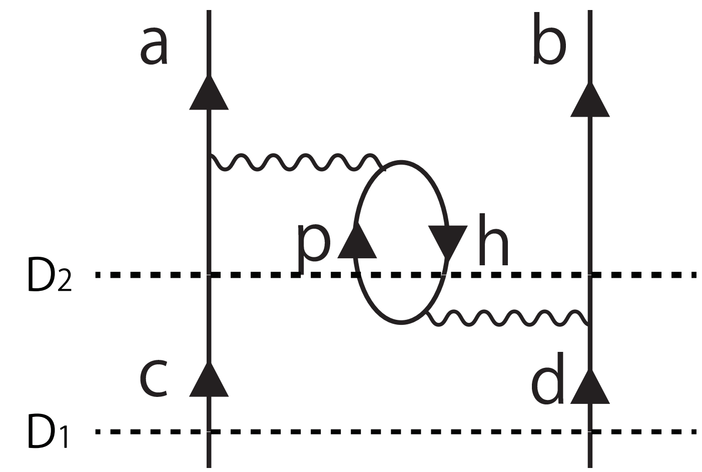
Example: EKK method avoids the divergences

EKK method



$$\frac{V_{ah,cp}V_{pb,hd}}{E - \epsilon_c - \epsilon_b - \epsilon_p + \epsilon_h}$$

KK method

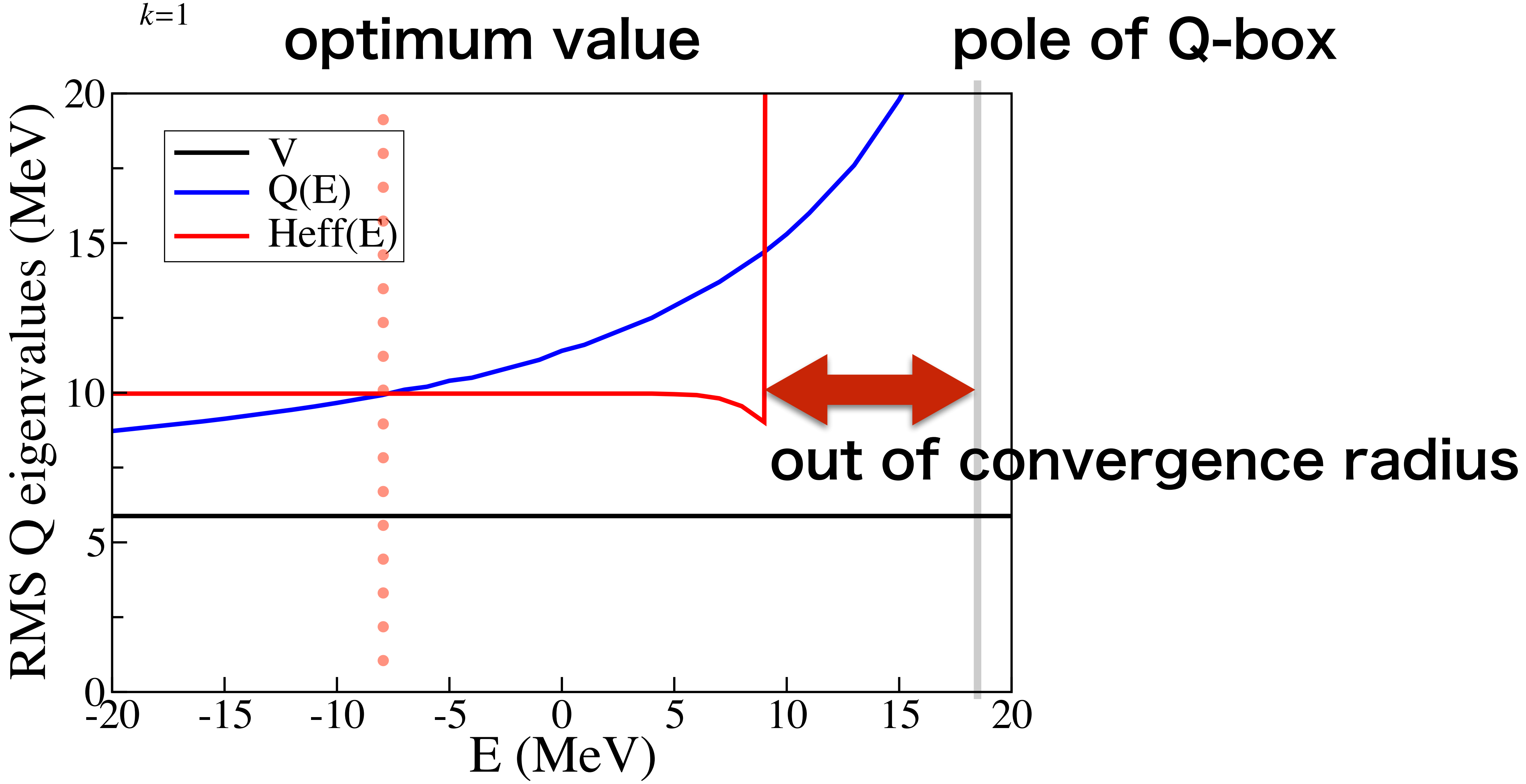


$$\frac{V_{ah,cp}V_{pb,hd}}{(\epsilon_c + \epsilon_d) - \epsilon_c - \epsilon_p + \epsilon_h - \epsilon_b}$$

- We can choose E to avoid divergence !
- Note that the choice of E is arbitrary and should give the same result if the Q-box is calculated without any approximation.
- Inversely, E-dependence is a **measure of error** coming from the approximation

E-depdence w and w/o non-perturbative correction

$$\tilde{H}_{\text{eff}}^{(n)} = \tilde{H}_{\text{BH}}(E) + \sum_{k=1}^{\infty} \hat{Q}_k(E)\{\tilde{H}_{\text{eff}}^{(n-1)}\}^k$$



★ Non perturbative correction vanishes the E-dependecne

★ Optimum value of E

EKK code algorithm

SPEs **TBMEs**

$$H = \sum_i \epsilon_i a_i^\dagger a_i + \sum_{ijkl} V_{ij,kl} a_i^\dagger a_j^\dagger a_l a_k.$$

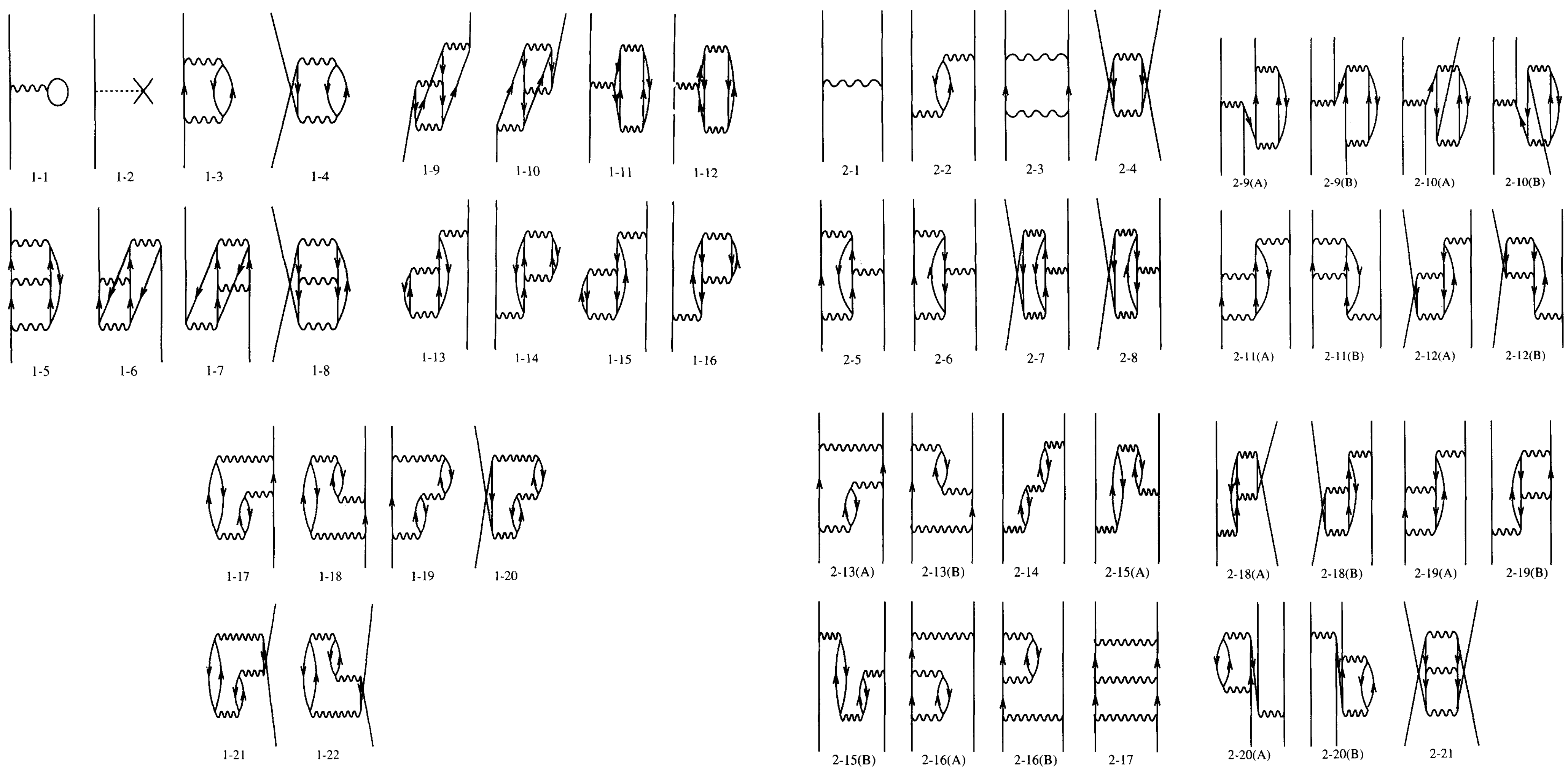
所要時間目安
(single node 換算)

read bare interaction from file	~10 s	
calculate SPEs ~ o(10) elements	~5 s	calculate ϵ_i
calculate TBMEs ~ o(10^2~10^4) elements	**10 h~100 days**	calculate $\hat{Q}_k(E)$
calculate folded diagrams	~5 s	iteration

$$\tilde{H}_{\rm eff}^{(n)} = \tilde{H}_{\rm BH}(E) + \sum_{k=1}^{\infty} \hat{Q}_k(E) \{\tilde{H}_{\rm eff}^{(n-1)}\}^k$$

EKK code algorithm

About 50 diagrams (76 tasks) to be calculated for **each** TBMEs (2116 for sdpf-shell, 6380 for pfsdg-shell)-> MPI parallel calculation (master-slave scheme)



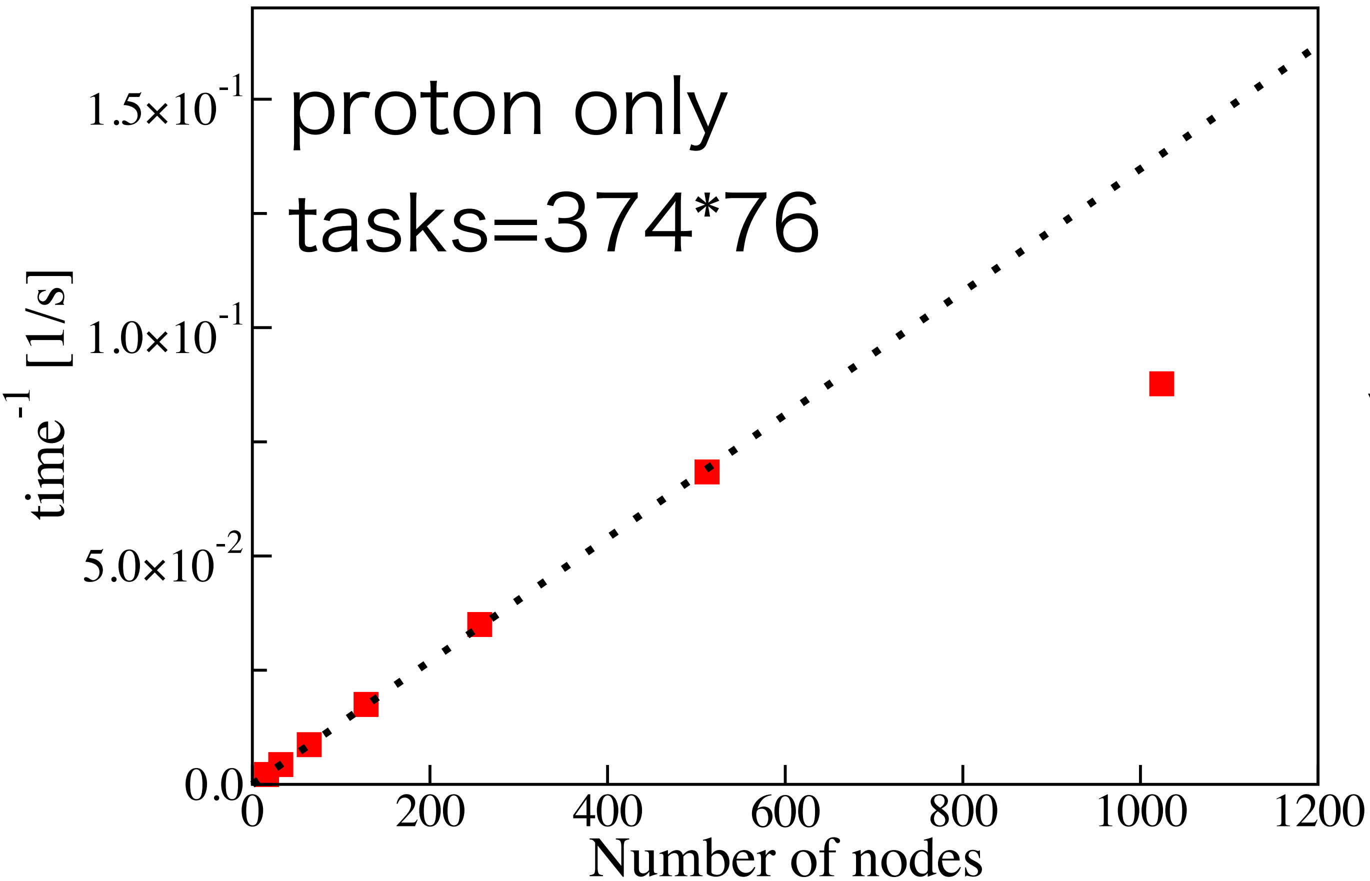
Each diagram -> openMP parallel calculation for particle loop

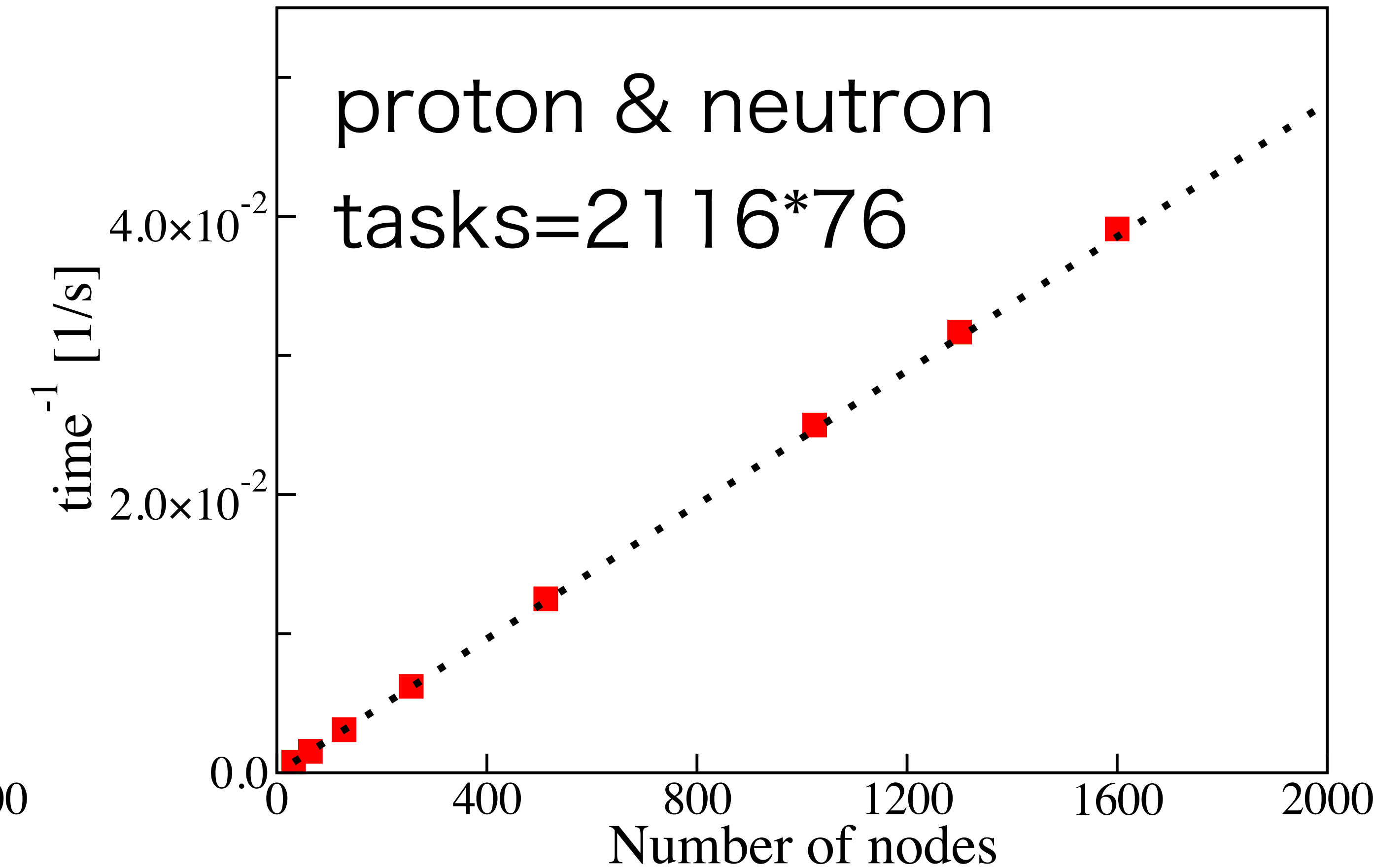
MPI+openMP scaling

Test case: sdpf-shell

13major shells

oakforest (64 core, max 2048 nodes)



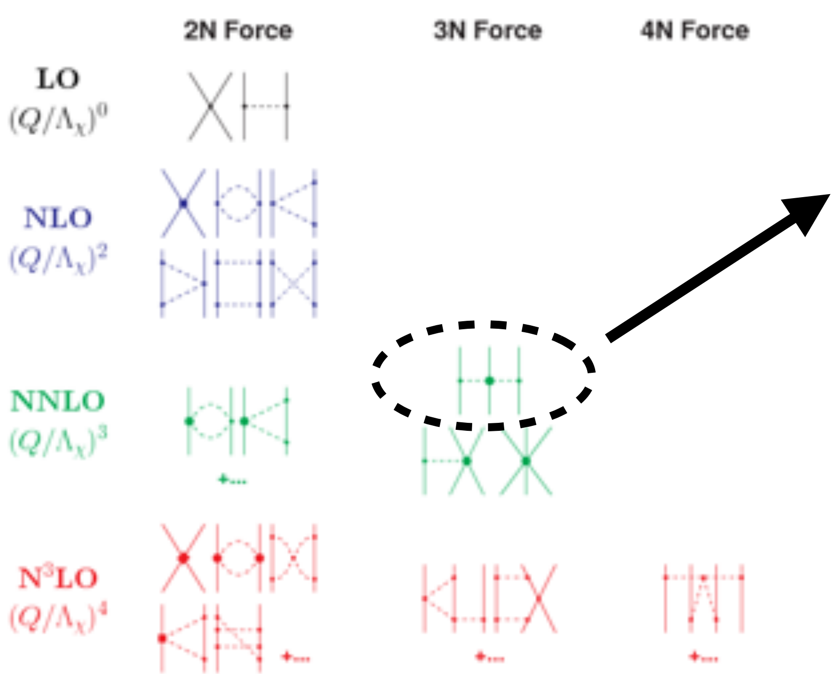


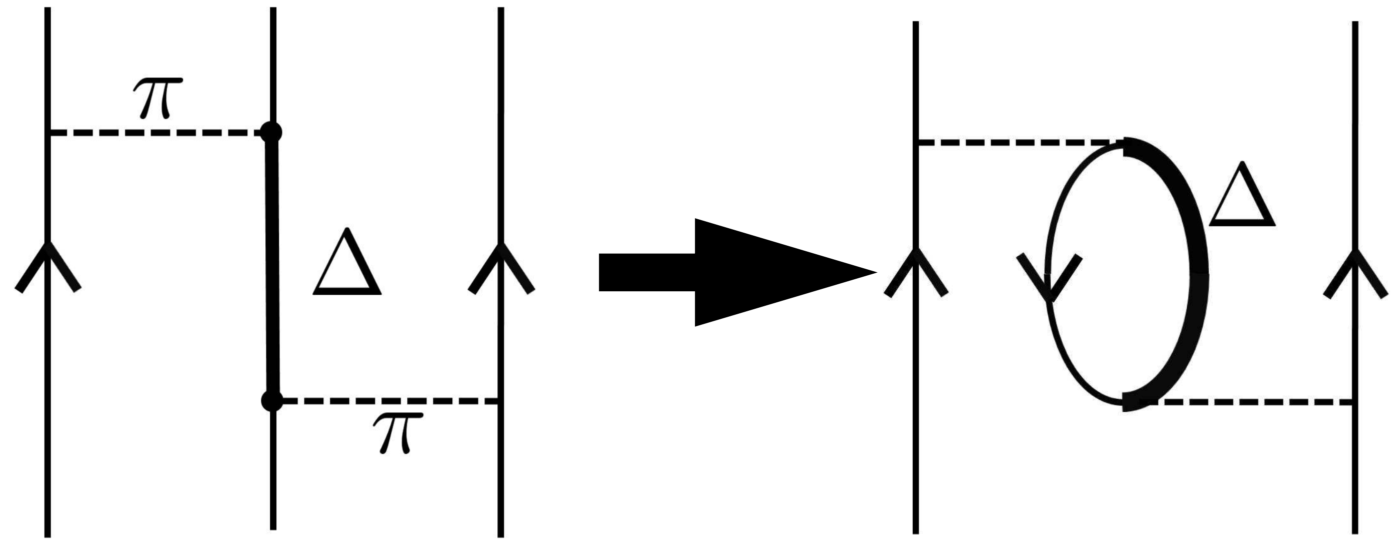
# of nodes ~ # of TBMEs までは良い効率で並列化可能
(グラフでは)

3N interaction (Δ-hole interaction)

summation with hole state

main contribution of 3N





Fujita-Miyazawa type
3N interaction

Effective
2N interaction

- Adding up effective 2N interaction derived from 3N interaction to EKK 2N effective interaction [1]
- This is one of the lowest order interaction from 3N force and for higher order we are working on…

[1] T. Otsuka, T. Suzuki, J. D. Holt, A. Schwenk, and Y. Akaishi, Phys. Rev. Lett. 105, 032501 (2010).

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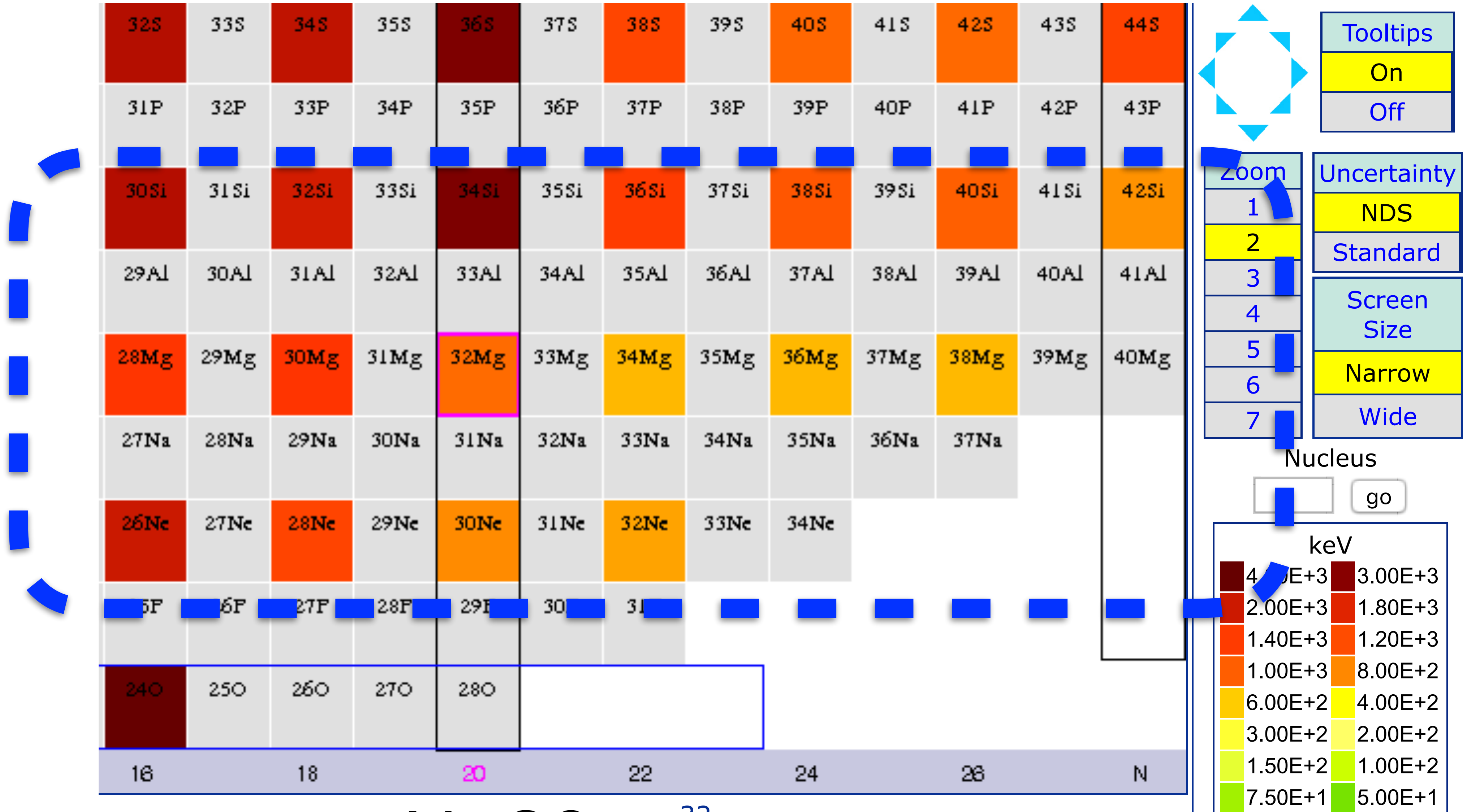
Island of inversion

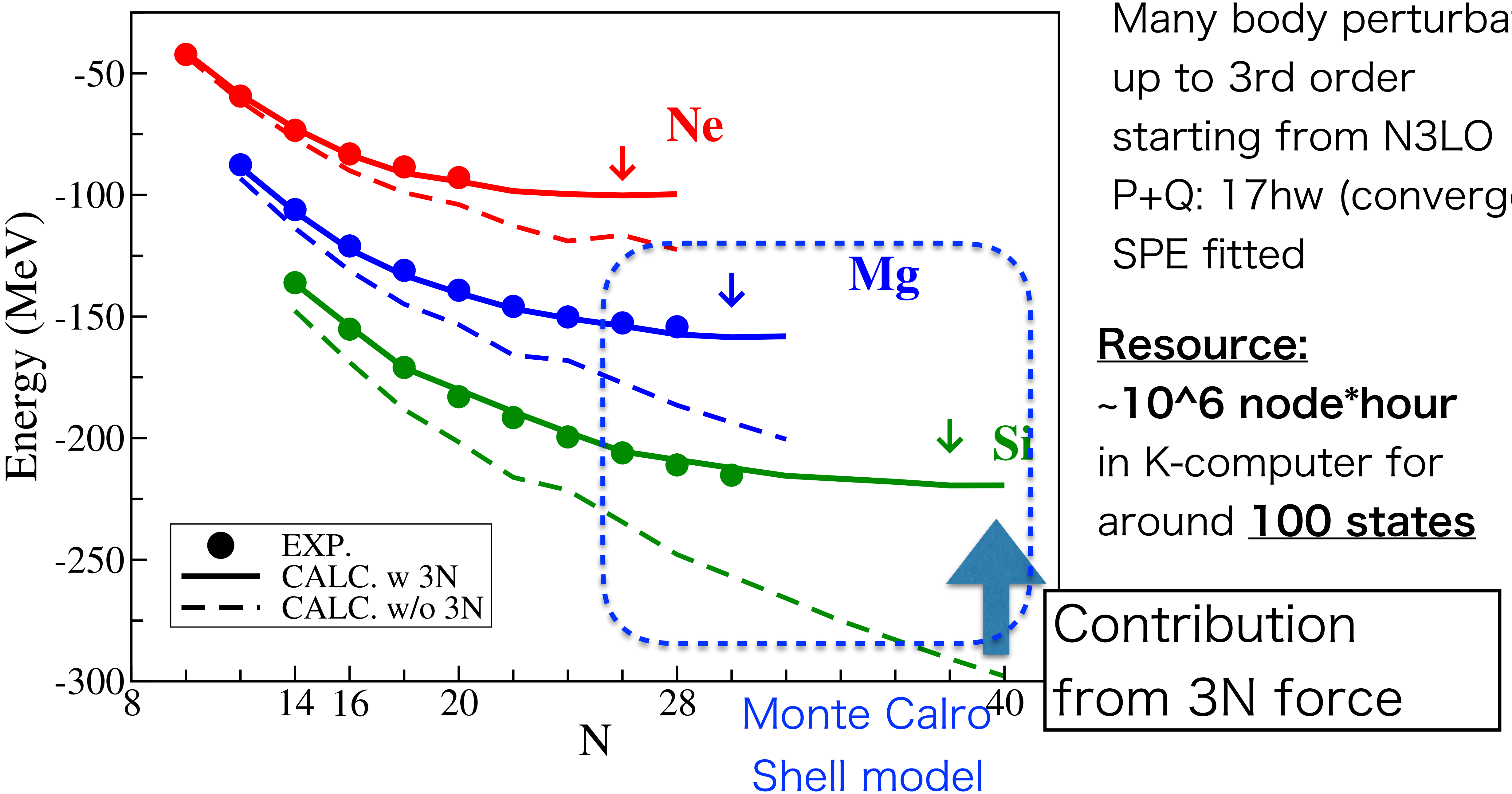
http://www.nndc.bnl.gov/nudat2/reCenter.jsp?z=12&n=20



N=20

- Around Ne and Mg region N=20 major gap disappears. (small 2+ energy for even-even nuclei, large deformation, etc…)
- Ground state is consist of “**inverse**” configuration, i.e. intruder configuration
- Can microscopic theory describe this disappearance of major magic number?

Ground state energies and dripline

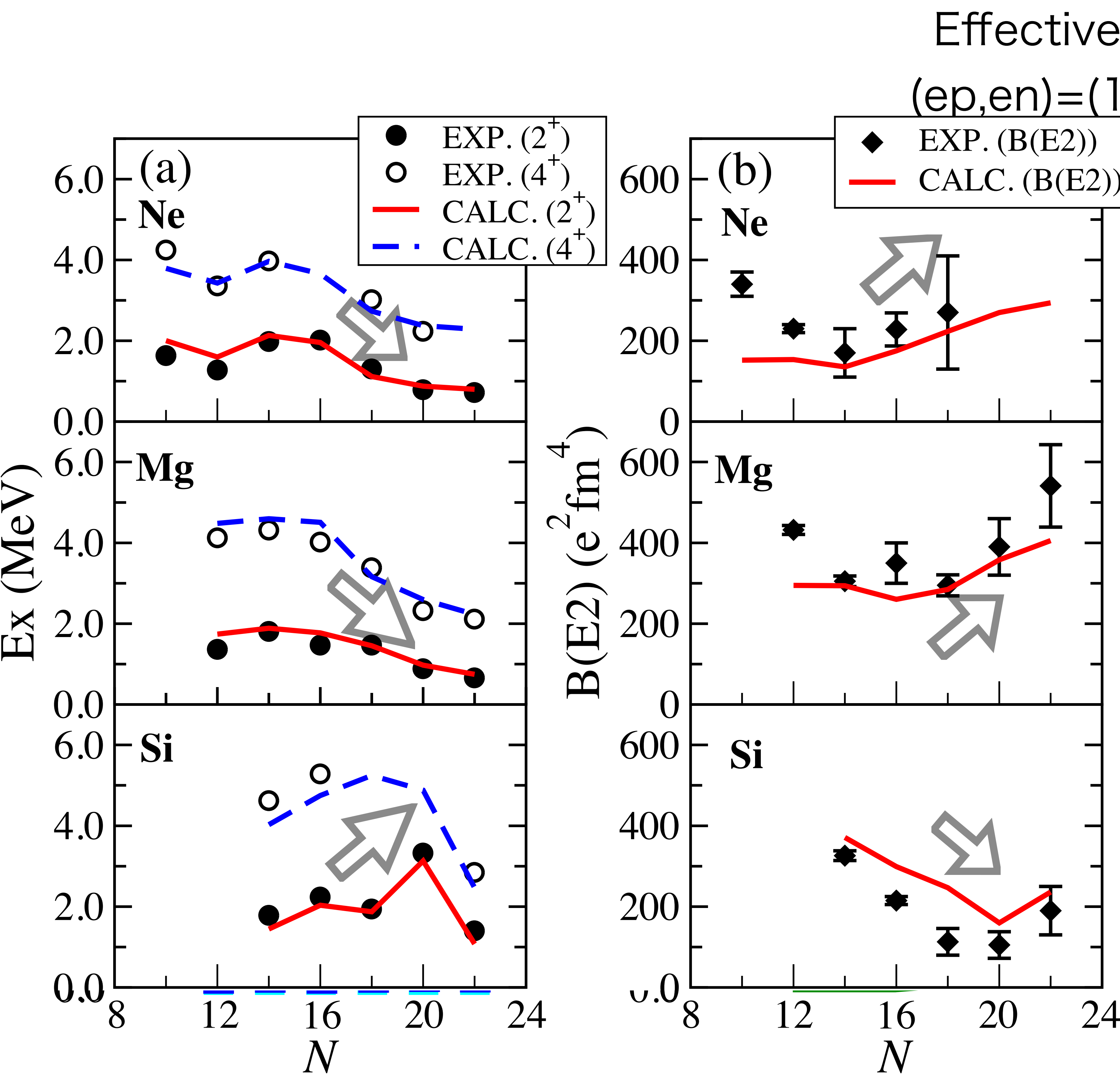


Many body perturbation up to 3rd order starting from N3LO
P+Q: 17hw (converged)
SPE fitted

Resource:
~10^6 node*hour
in K-computer for around **100 states**

- Contribution of 3N force is significant in neutron-rich nuclei
- Predictions of dripline
- Combination of **Microscopic theory** and **Large scale calc.**

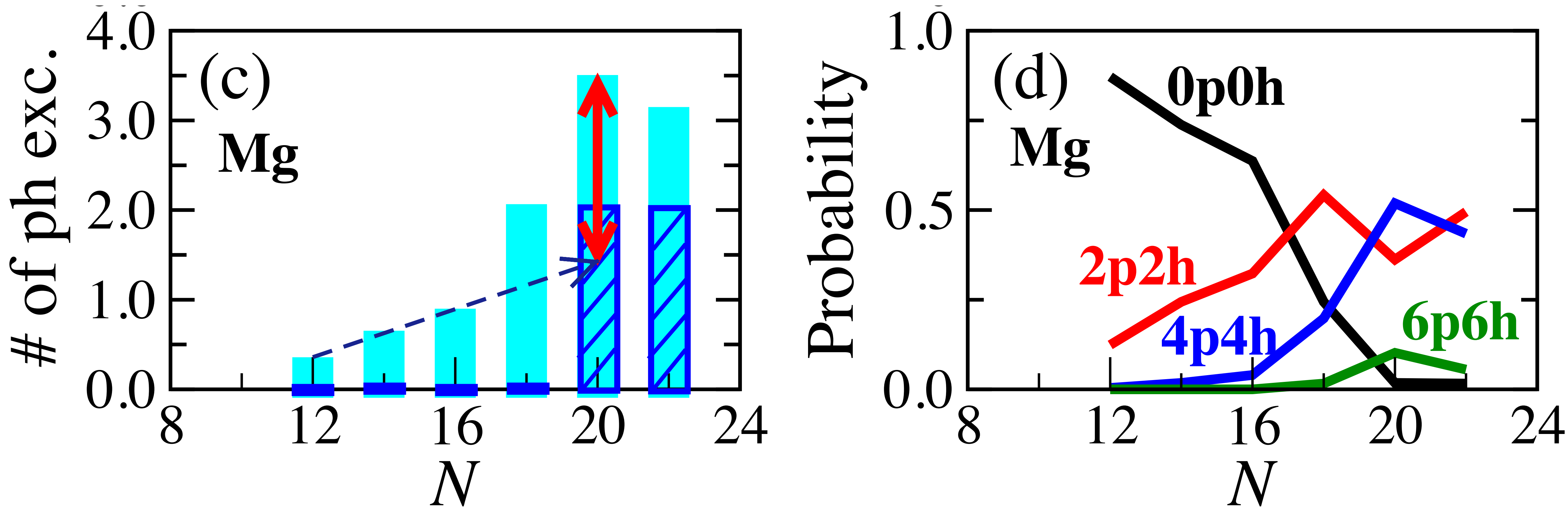
Shell structure in “island of inversion”



Clear indication of breaking of N=20 gap for Ne and Mg.

N=20 gap remains in Si case.

Wave function of Mg isotopes



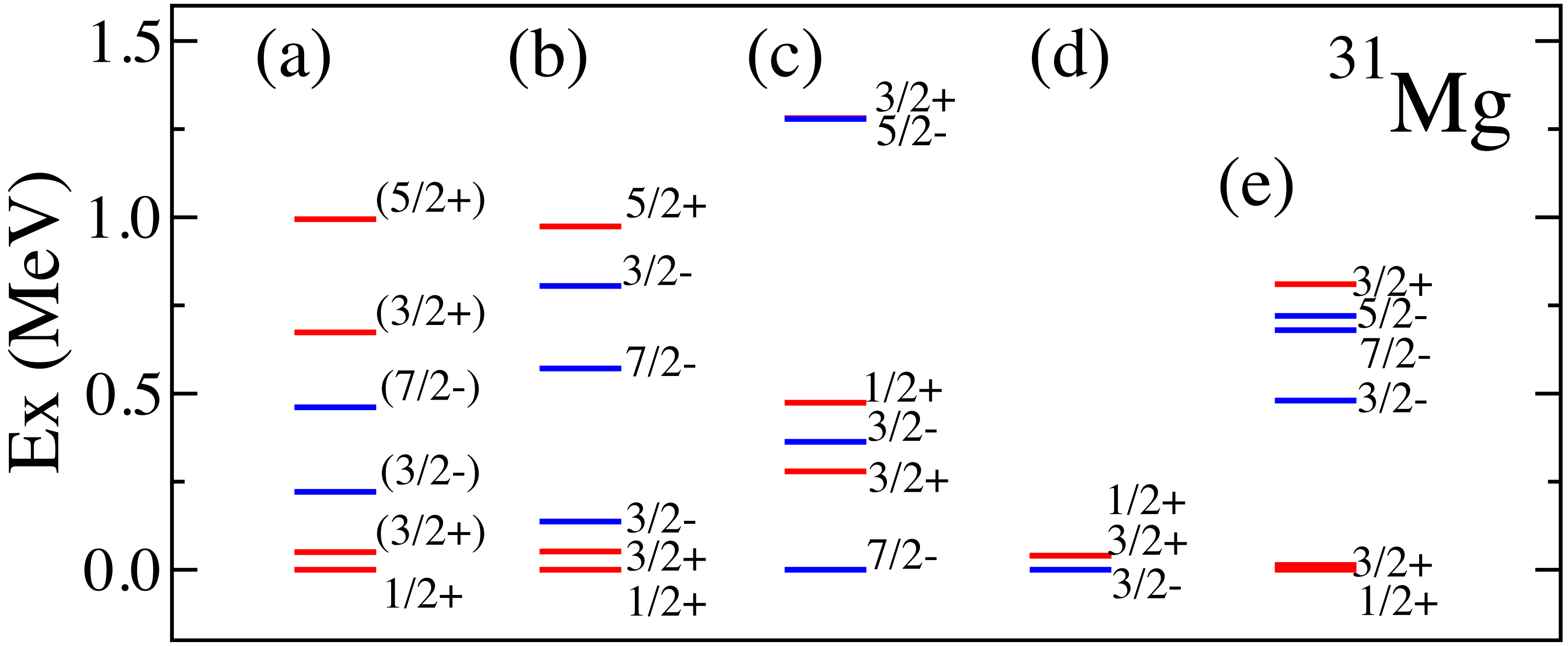
<u>"modest" and "abrupt" excitation</u>

modest: shifting between two shells (e.g. pairing)

abrupt : strong deformation

Abrupt excitation roughly corresponds to conventional 2p2h excitation model

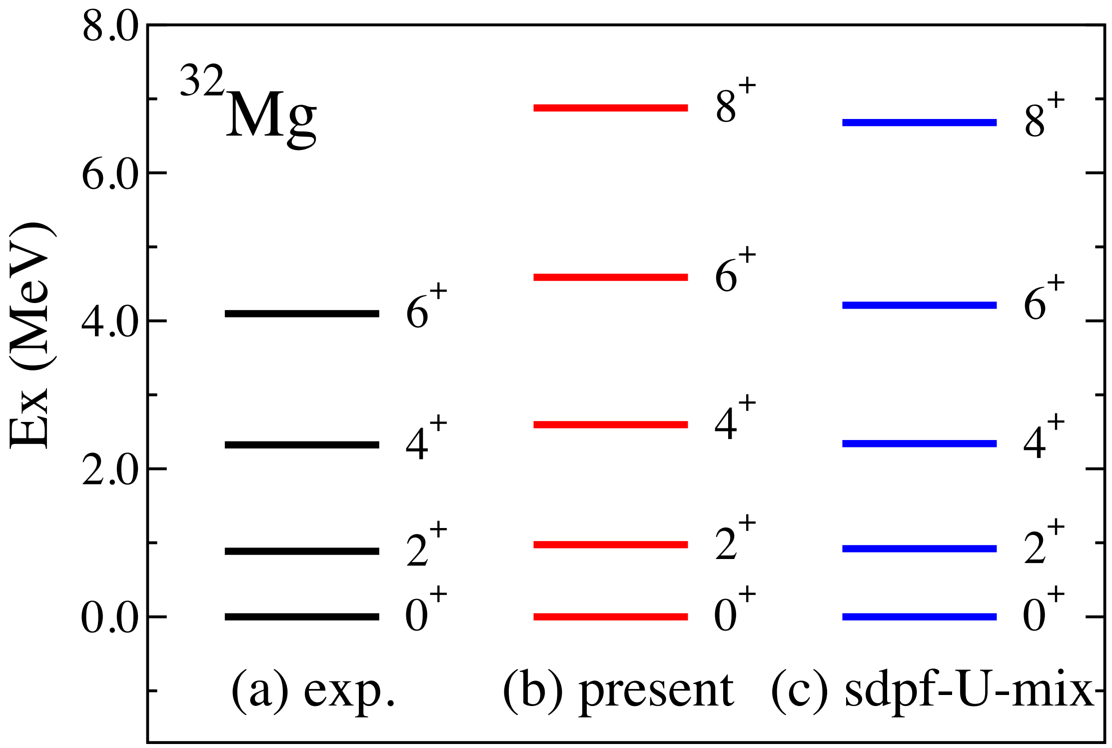
31Mg



(a) EXP.
(b) EKK+3N
(c) sdpf-m (phenom.)
(d) sdpf-U-mix (phenom.)
(e) AMD+GCM

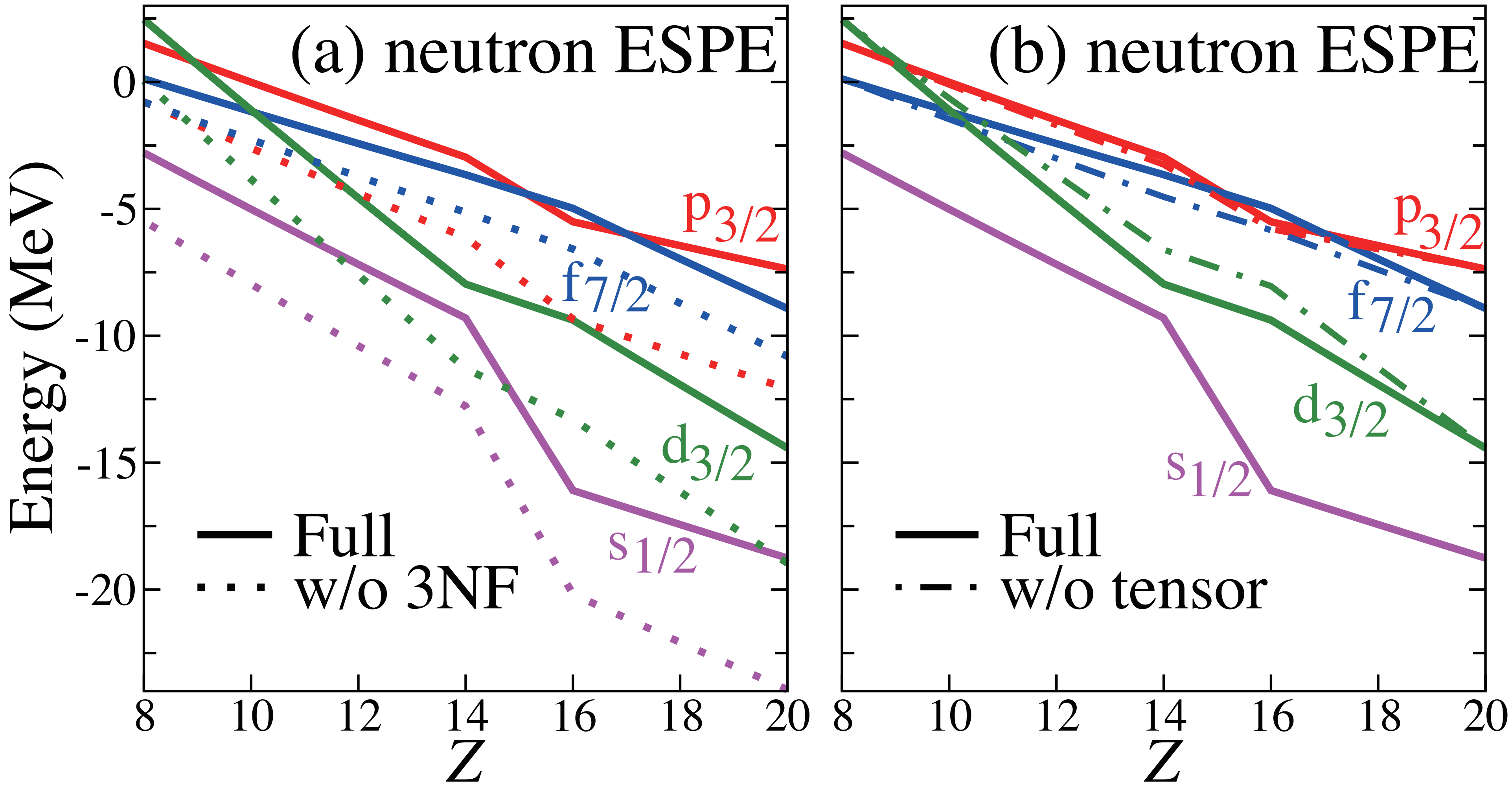
- onset of island of inversion
- ordering of levels reproduced
- positive=2hw dominanted
- negative=1hw dominated

<u>Deformation of 32Mg</u>



Evolution of single particle states

Effective single particle energies at N=20 isotones



3NF: general shift

Tensor force: drive sd to pf gap

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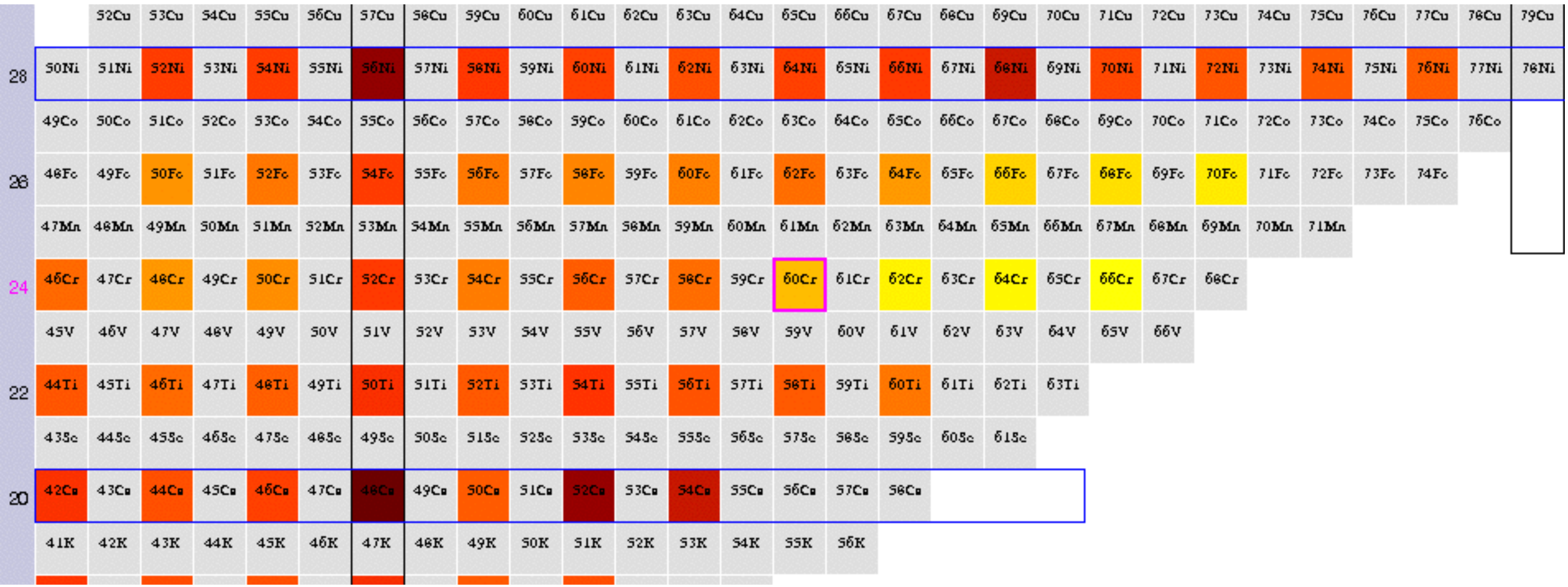
Ca~Ni isotopes, several magic numbers

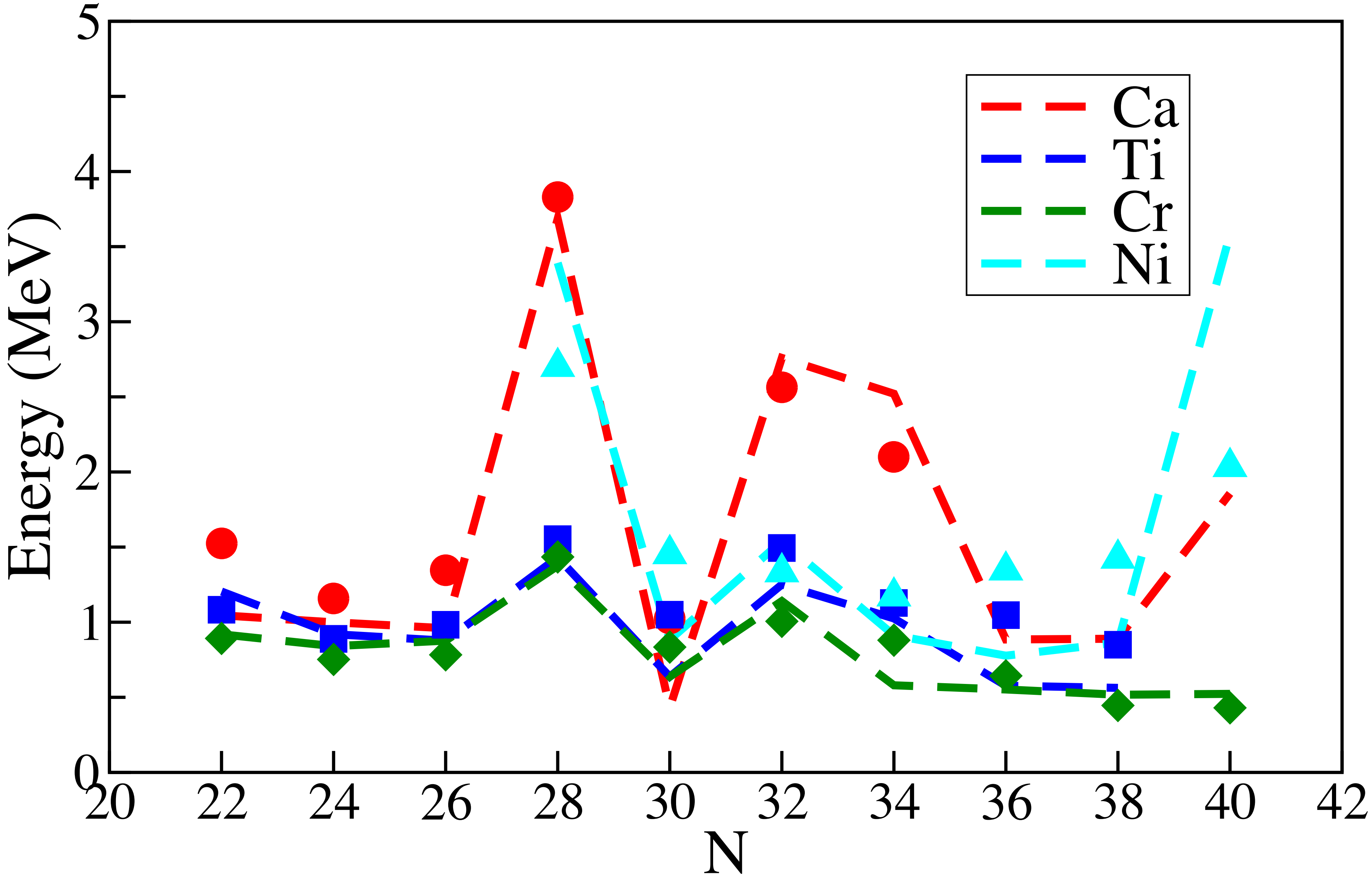
E2+ of even-even isotopes



N=28 32 34 40 50

- “Second” island of inversion
- Wider area, larger calculations (ポスト京に向けて)

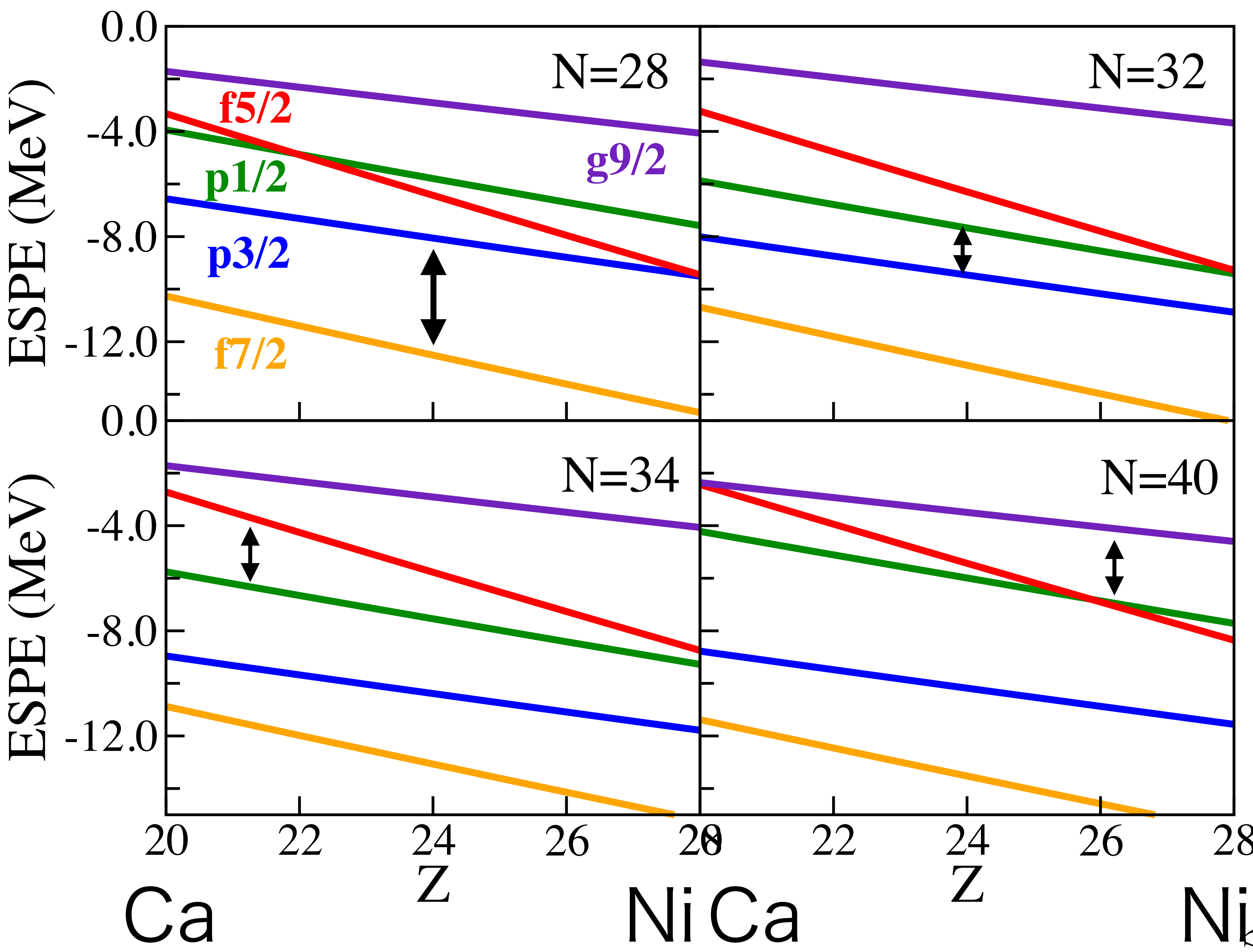
E^{2+} of Ca, Ti, Cr and Ni isotopes (preliminary)



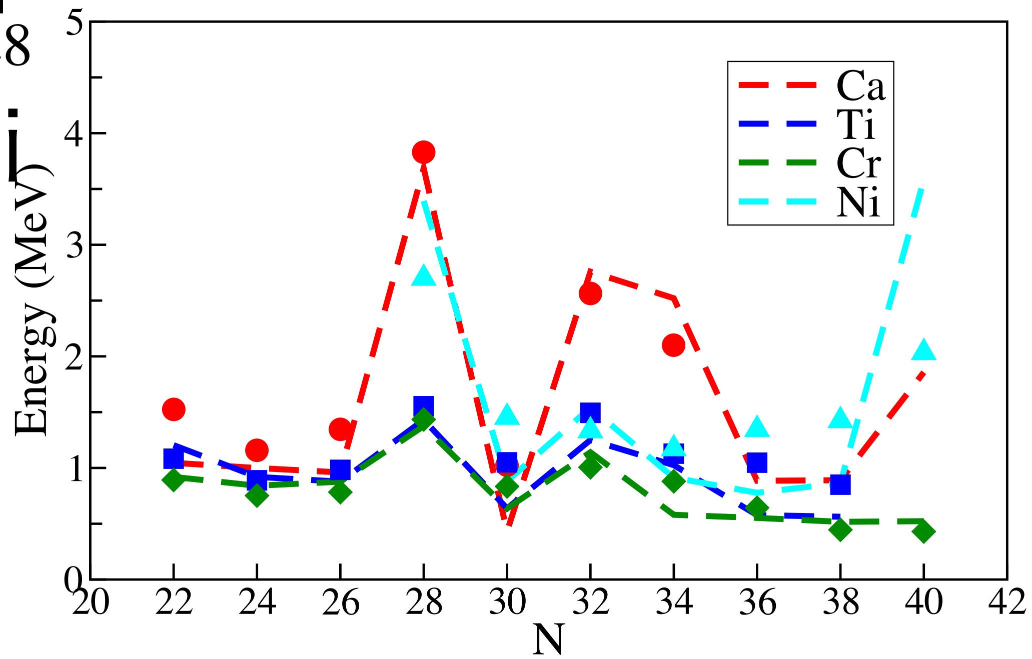
Interaction
pf+sdg-shell
P+Q: 13 major shell
vlowk + 3NF(FM)
3rd order perturbation
6380 TBMEs
500 node*h in K

Appearance and disappearance of N=28, 32, 34, 40 magic numbers

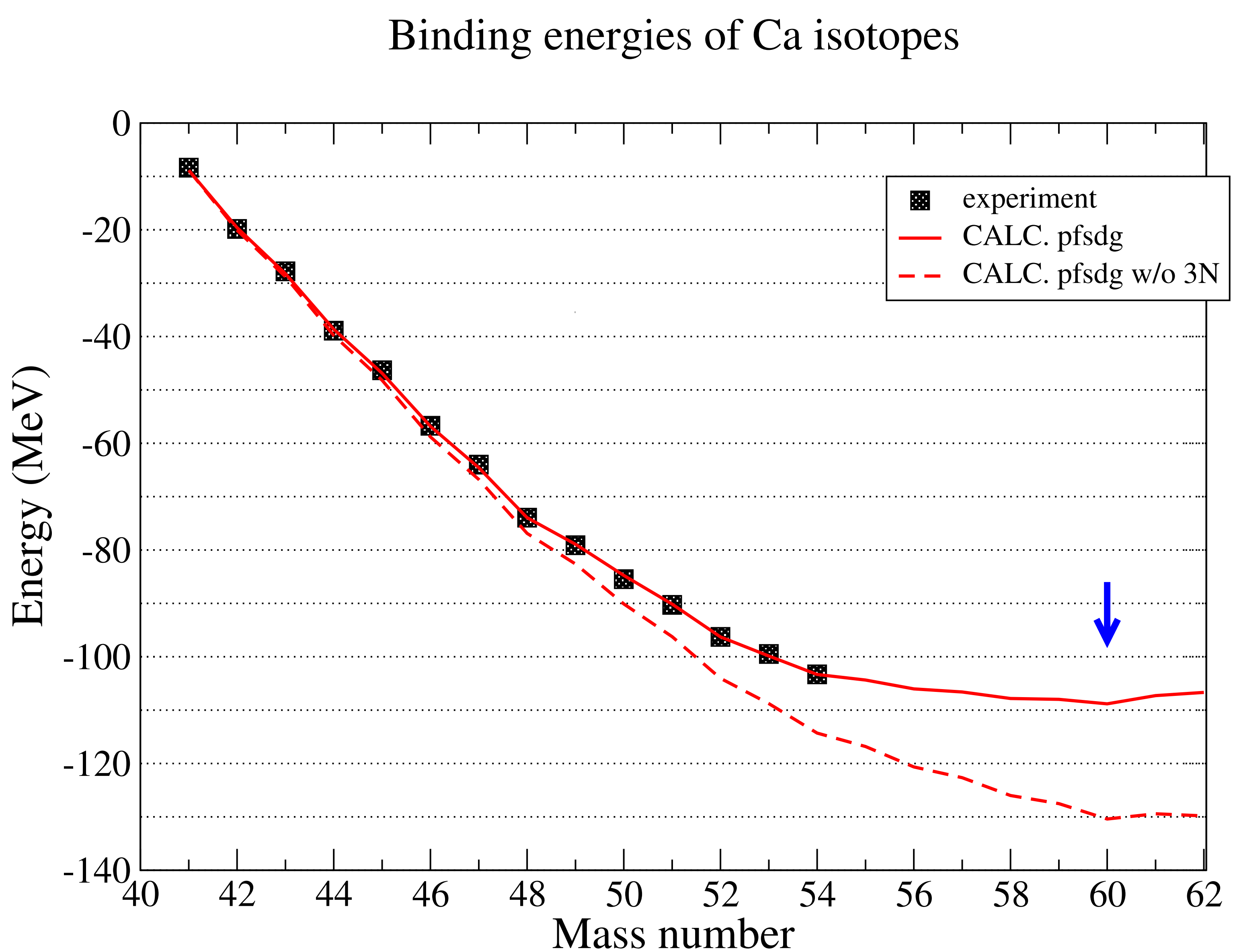
Evolution of single particle states



N=28, 32 gap looks stable comparing to N=34,40 gap



Binding energy and 3N force (preliminary)



3NF is important for binding energy, in the same way as in the case of sdpf-shell

Future direction

pf+sdg-shell の計算は、ある程度小規模の計算により、うまくいきそうなことが分かった段階。

今後と課題

1. 三体力の扱い
   - Fujita-Miyazawa type だけでなく、カイラル摂動論に基づいた他の方法
   - 摂動論の基底の変換(Hartree-Fock basis)
2. EKK 計算を精密化
   - テストケースでは、13 major-shell だったが、収束にはもう少し必要　→　ポスト京に向けて、コードをさらに高速化

Summary and conclusion

- MBPT is the theory to construct the effective Hamiltonian starting from nuclear force.
- EKK method is introduced to derive the effective interaction for the shell model which is applicable to **multi-shell** system.
- As an application of EKK method, the physics in the **“island of inversion”** is discussed in K-computer.
- As a future project, physics in pf+sdg-shell is discussed with preliminary results.
- **EKK** and **3N** combination is the powerful tool to explore the wide area of the nuclear chart

Collaborators

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- Toshio Suzuki (Nihon Univ.)
- Morten Hjorth-Jensen (Oslo Univ.)