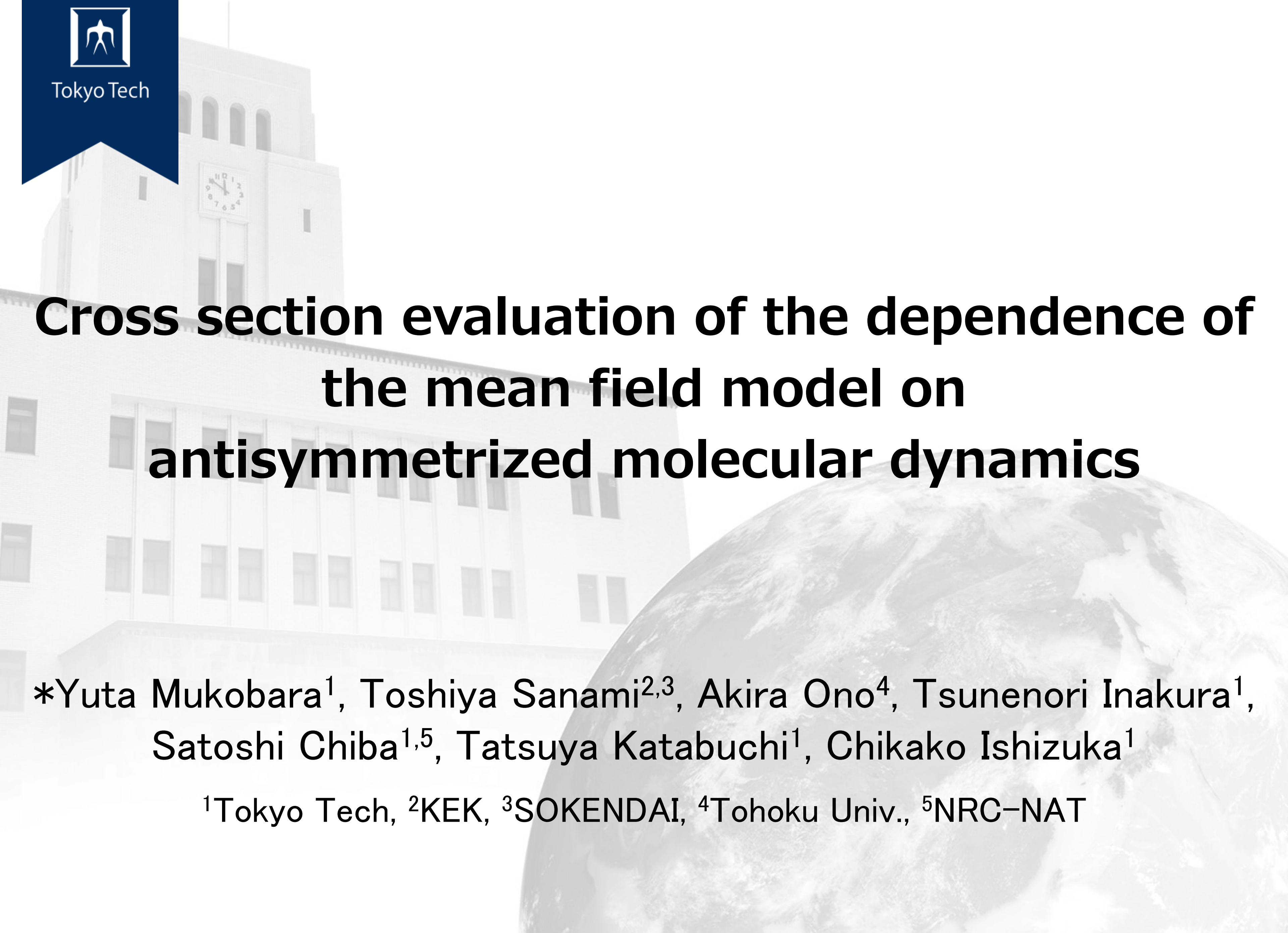

Cross section evaluation of the dependence of the mean field model on antisymmetrized molecular dynamics

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Contents

Background & Purpose

Difficulties in heavy-ion nuclear reactions

- ^{12}C-induced reactions at MeV order energy are important not only in astronomical contexts but also in applications such as cancer therapy, thanks to recent advances in accelerator technology.

- However, compared to light-ion nuclear reactions, heavy-ion nuclear reactions have a more complex reaction mechanism, and thus a theoretical framework for calculation has not been established. Therefore, models based on various assumptions are used depending on the conditions (e.g., incident energy, impact parameter and reaction system).

Why ^{12}C–induced reaction?

- **Astrophysics**

  Nuclear reactions at MeV order energy of ^{12}C+^{16}O can efficiently make ^{20}Ne at MeV order energy. It has been suggested that this could have implications for supernova explosion scenarios, such as regulating the burning rate of carbon in stellar interiors.

- **Nuclear Physics**

  In the field of nuclear physics, the alpha cluster structure is known as a nuclear structure. Recently, the existence of deuteron clusters has also been actively studied as a nuclear structure[1].

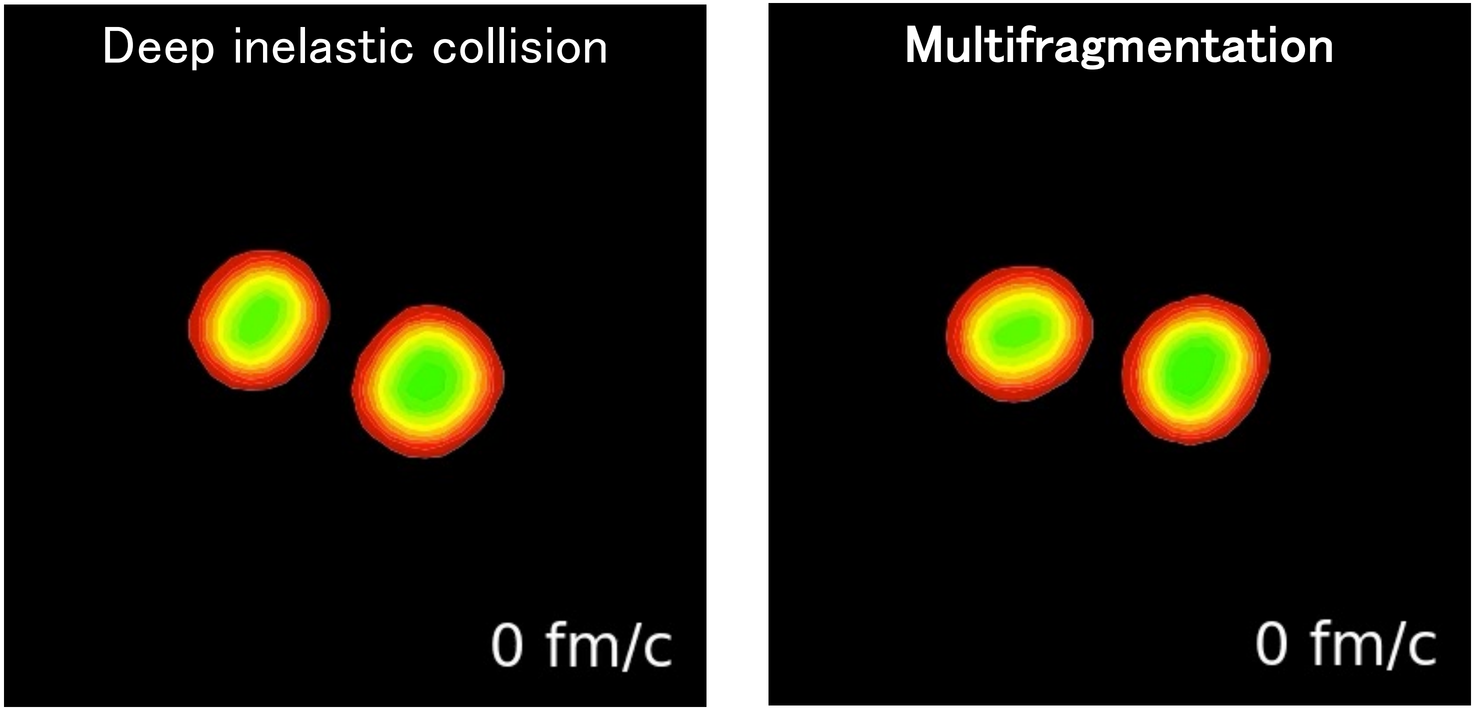
^{12}C is also an important nuclide in the nuclear structure field because of its potential to produce deuteron clusters.

[1] Y. Chazono *et al.* Phys. Rev. C 106, 064613 (2022)

AMD simulation of ^{12}C + ^{16}O reaction

Reaction Systems for Heavy Ion Cancer Therapy

^{12}C + ^{16}O reaction at 100 MeV/u



The purpose of this study is to quantify the dependence of the AMD on the mean field for the calculation of production cross sections in the ^{12}C–induced reaction used in cancer therapy.

- Evaluate the accuracy of calculations of heavy–ion reactions.
- Elucidate the causes of mean–field dependence in mean–field models.

Method

Theory of AMD

Single-particle wave function:

Gaussian wave packet

$$\langle \boldsymbol{r} | \varphi_i \rangle = \left(\frac{2\nu}{\pi} \right)^{3/4} \exp \left[-\nu \left(\boldsymbol{r} - \frac{\boldsymbol{Z}_i}{\sqrt{\nu}} \right)^2 \right] \chi_i$$

$$\boldsymbol{Z}_i = \sqrt{\nu} \boldsymbol{R}_i + \frac{i}{2\hbar\sqrt{\nu}} \boldsymbol{P}_i$$

Total wave function:

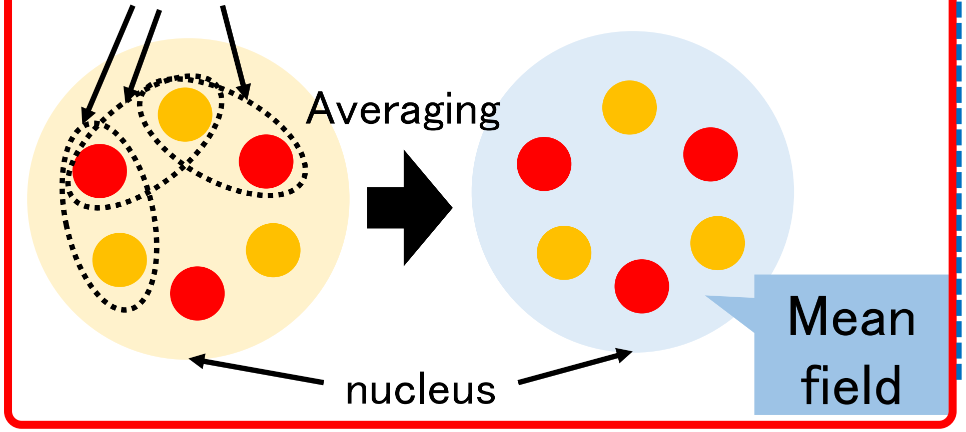
Slater determinant

$$|\Phi(r_1, r_2, \cdots, r_A)\rangle = \frac{1}{\sqrt{A!}} \det [\varphi_i(r_j)]$$

Mean-field effects

● ● } nucleon (p・n)

Interaction between two nucleons



Equation of motion

$$0 = \delta \int_{t_1}^{t_2} \mathrm{d}t \frac{\langle \Phi(\mathbf{Z}) | i\hbar(\frac{d}{dt}) - \hat{H} | \Phi(\mathbf{Z}) \rangle}{\langle \Phi(\mathbf{Z}) \mid \Phi(\mathbf{Z}) \rangle}$$

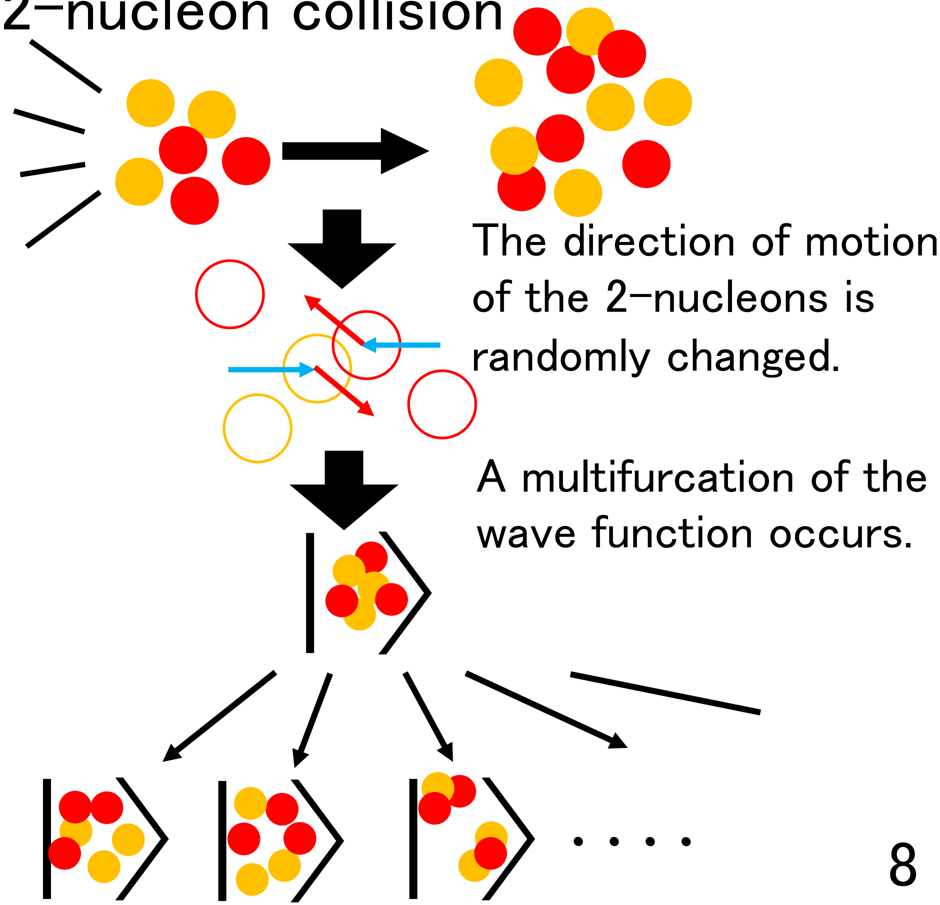
Hamiltonian $\hat{H}$

$$\hat{H} = \sum_{i=1}^{A} \hat{t}_i + \sum_{i<j=1}^{A} \hat{v}_{ij}$$

kinetic energy operator: $\hat{t}_i$

effective interaction: $\hat{v}_{ij}$

2-nucleon collision



The direction of motion of the 2-nucleons is randomly changed.

A multifurcation of the wave function occurs.

Mean field model to be used

Various effective interactions have been proposed, including Skyrme force used in this work

$$\begin{aligned}
V_{ij} = {} & t_0(1+x_0P_\sigma)\delta(\boldsymbol{r}_i-\boldsymbol{r}_j) && \cdots \text{ S−wave component (attractive force)}\\
& +\frac{1}{2}t_1(1+x_1P_\sigma)\left[\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\boldsymbol{k}^2+\boldsymbol{k}'^2\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\right] && \cdots \text{ P−wave component (surface effect)}\\
& +t_2(1+x_2P_\sigma)\boldsymbol{k}'\cdot\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\boldsymbol{k} && \cdots \text{ P−wave component (surface effect)}\\
& +\frac{1}{6}t_3\rho^\alpha\left(\frac{\boldsymbol{r}_i+\boldsymbol{r}_j}{2}\right)(1+x_3P_\sigma)\delta(\boldsymbol{r}_i-\boldsymbol{r}_j) && \cdots \text{ Multi−body force (repulsion)}\\
& +iW_0(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j)\cdot\left[\boldsymbol{k}'\times\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\boldsymbol{k}\right] && \cdots \text{ Spin−orbit force}
\end{aligned}$$

$$P_\sigma = \frac{1+\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j}{2} \quad \cdots \text{ Spin exchange operator}$$

$$\left.\begin{aligned}
\boldsymbol{k} &= \frac{\overrightarrow{\nabla}_i-\overrightarrow{\nabla}_j}{2i}\\
\boldsymbol{k}' &= -\frac{\overleftarrow{\nabla}_i-\overleftarrow{\nabla}_j}{2i}
\end{aligned}\right\} \cdots \text{ Relative momentum}$$

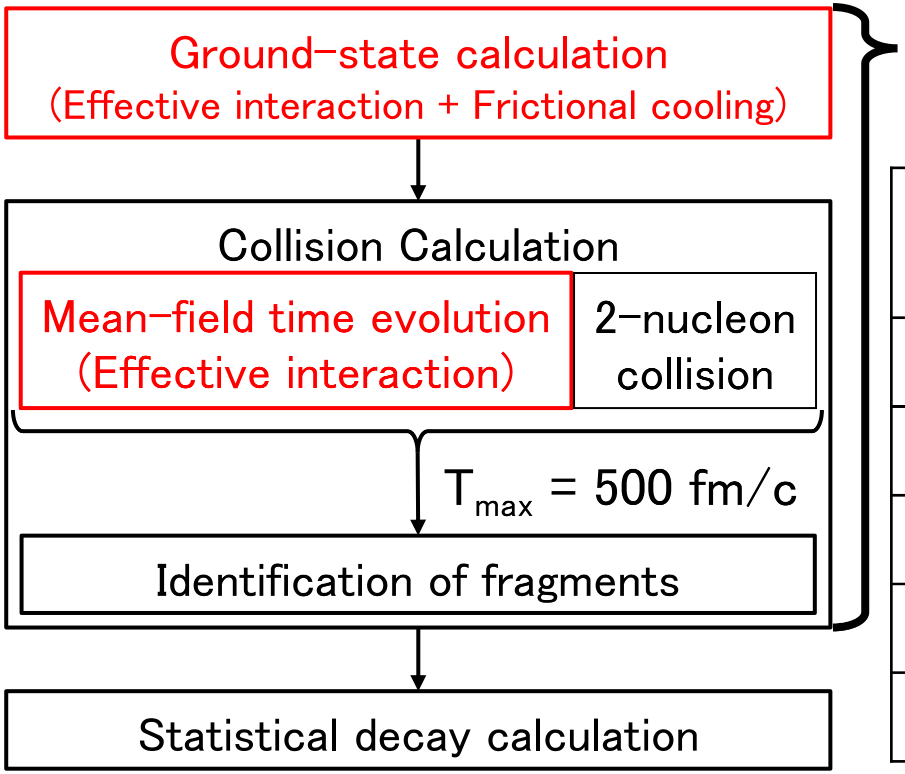
Effective interaction
(Skyrme force)

SLy4	SLy5_min
SkM*	SkI3
KDE	

Calculation details

How the calculation proceeds

1. Prepare ground states. → Frictional cooling by using 5 different Skyrme forces.
2. Projectile is boosted toward target.
3. If 2-nucleon collision is to take place, momentum of the 2 nucleons are changed randomly. The Pauli blocking is checked after each 2-nucleon collision.
4. Remaining fragments are identified, and their excitation energy and angular momentum are calculated.
5. Statistical decay calculations based on Hauser-Feshbach theory.



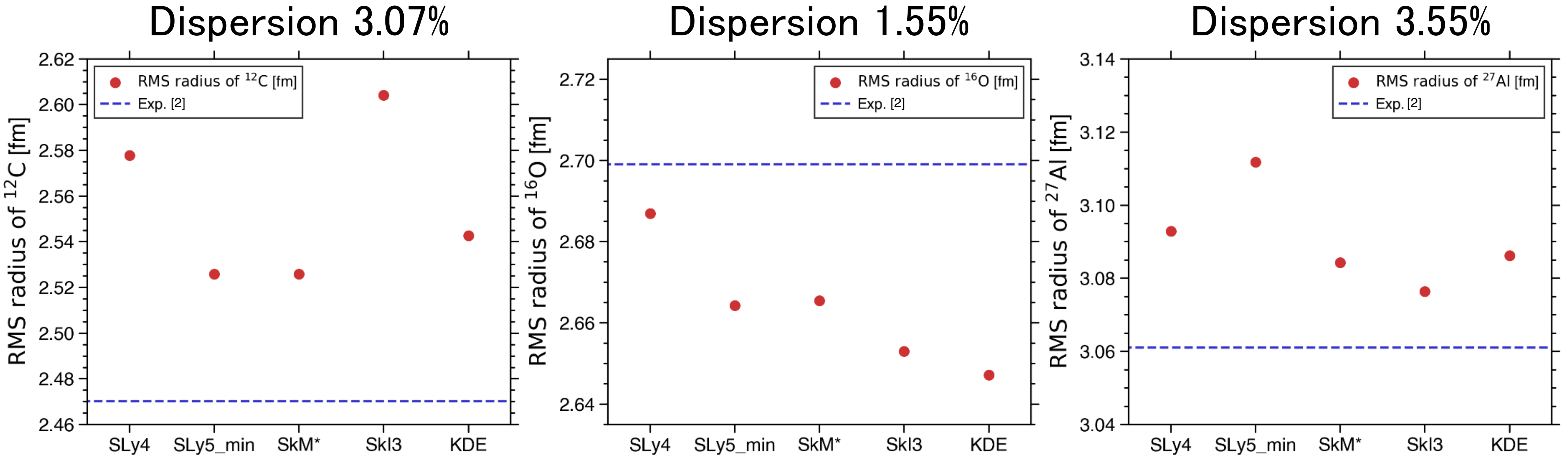
AMD

The reaction systems in this study

Projectile	Target	Incident energy	Number of events
^{12}C	^{16}O	72MeV	100,000
^{12}C	^{16}O	1200MeV	100,000
^{12}C	^{27}Al	72MeV	100,000
Proton	^{12}C	256 MeV	150,000
Proton	^{27}Al	256 MeV	150,000

Result

Cross section assumed from RMS radius



Dispersion 3.07%

Dispersion 1.55%

Dispersion 3.55%

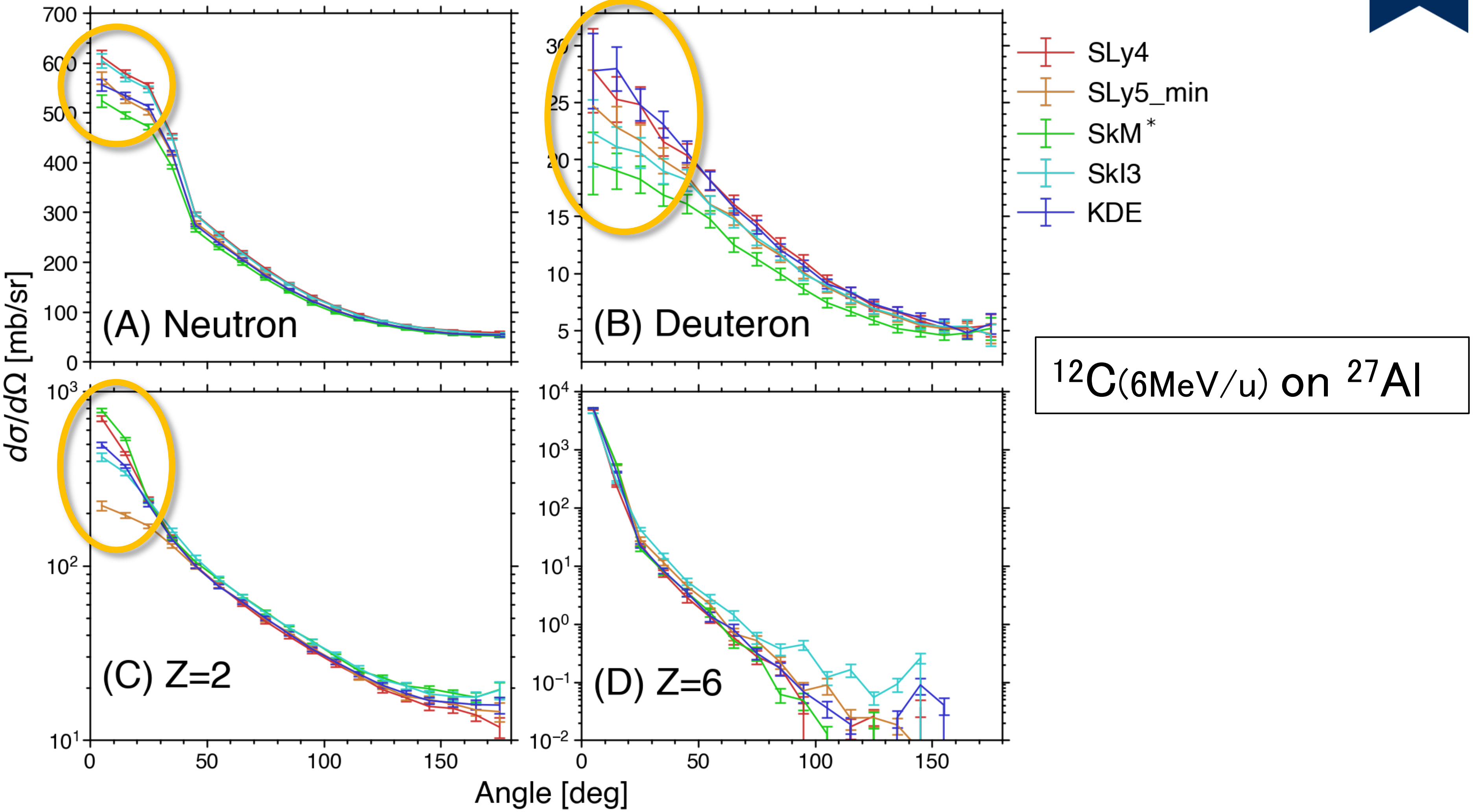
- Cross section depends on RMS radius
- The variation in the effective interaction handled in this case is about 3%

Based on the variation in RMS radius, the geometric cross section should have a variation of about 6.14% for ^{12}C and 3.10% for ^{16}O and 7.10% for ^{27}Al.

If the variation in reaction cross section is of this magnitude, it is reasonably understandable.

[2] I. Angeli *et al.* At. Data Nucl. Data Tables 99, 69 (2013)

Angular distribution



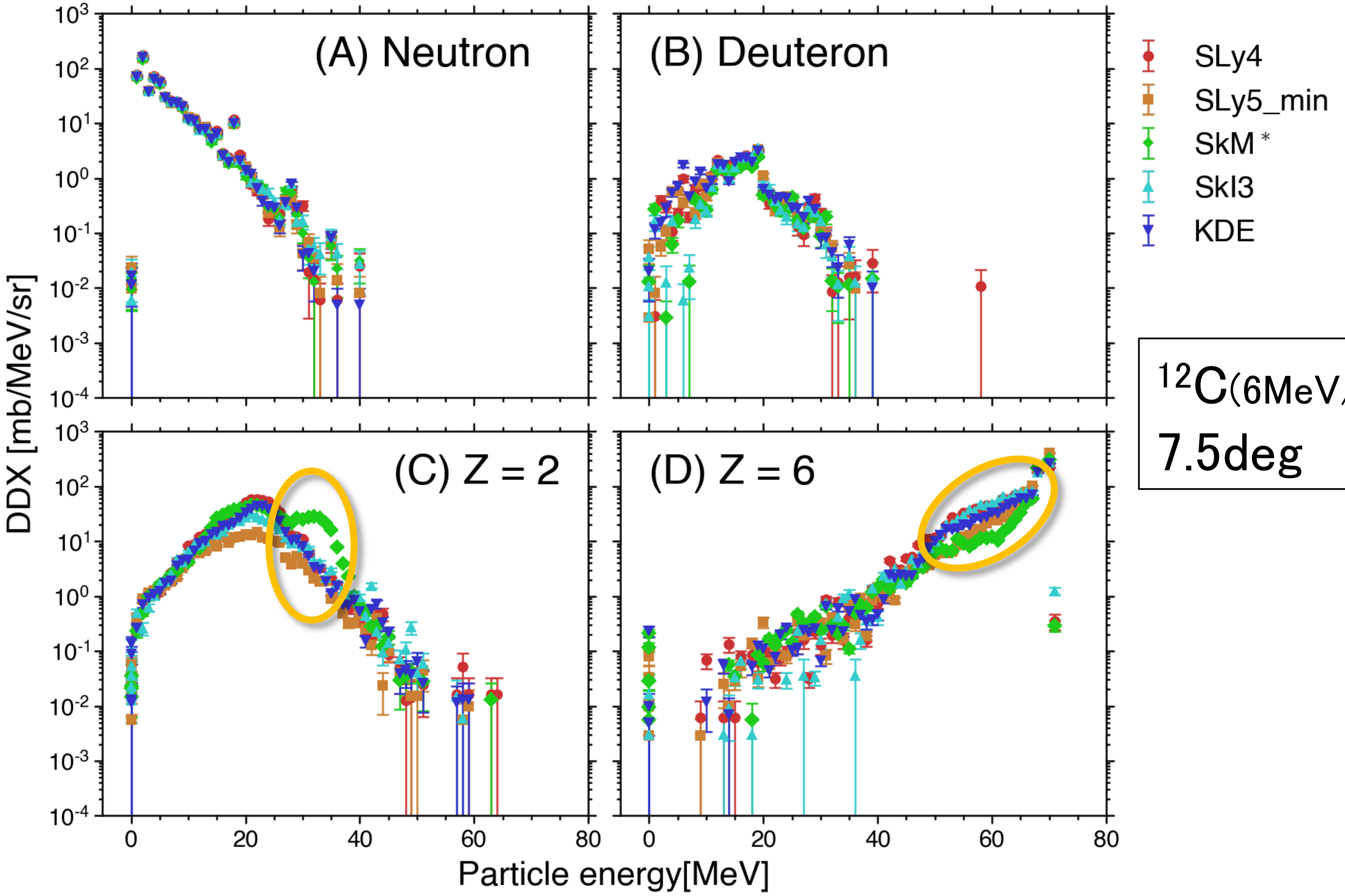
For neutron, the cross sections for SLy4 and SkI3 are large. For Deuteron, SLy4 and KDE are large. For Z=2, SLy4 and SkM* are large.

Thus, the mean-field model that gives the largest cross-section in each panel is different.

The mean-field effect is significant for forward emitted particles.

→ In the followings, we compare results such as DDXs at forward angles.

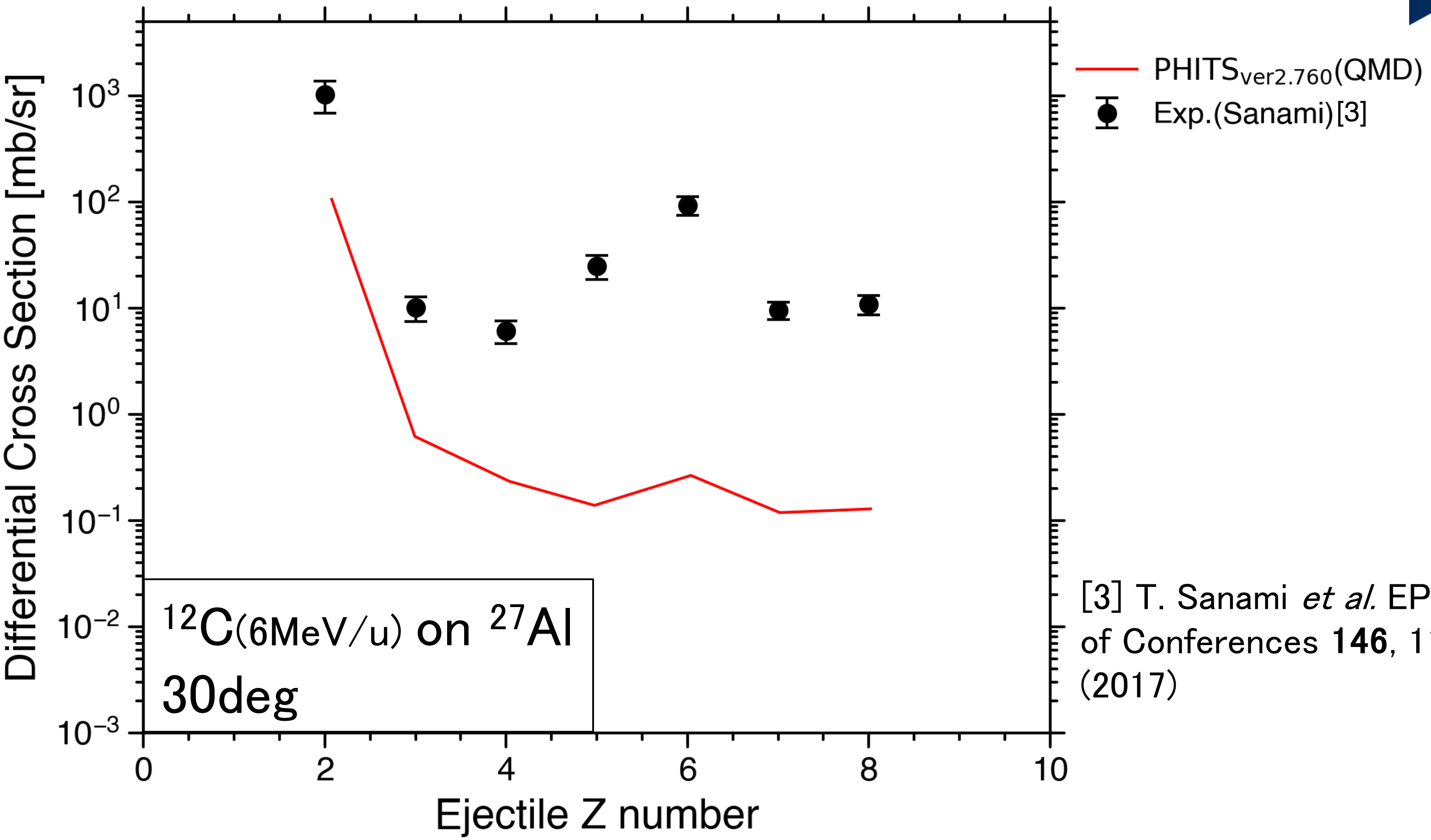
Comparison by DDX (1)



^{12}C(6MeV/u) on ^{27}Al
7.5deg

- There is a pronounced anomaly around 40 MeV in the helium isotope panel.
- The influence in carbon isotopes was also larger, and the influence was more pronounced in the higher energy portions above 50 MeV.

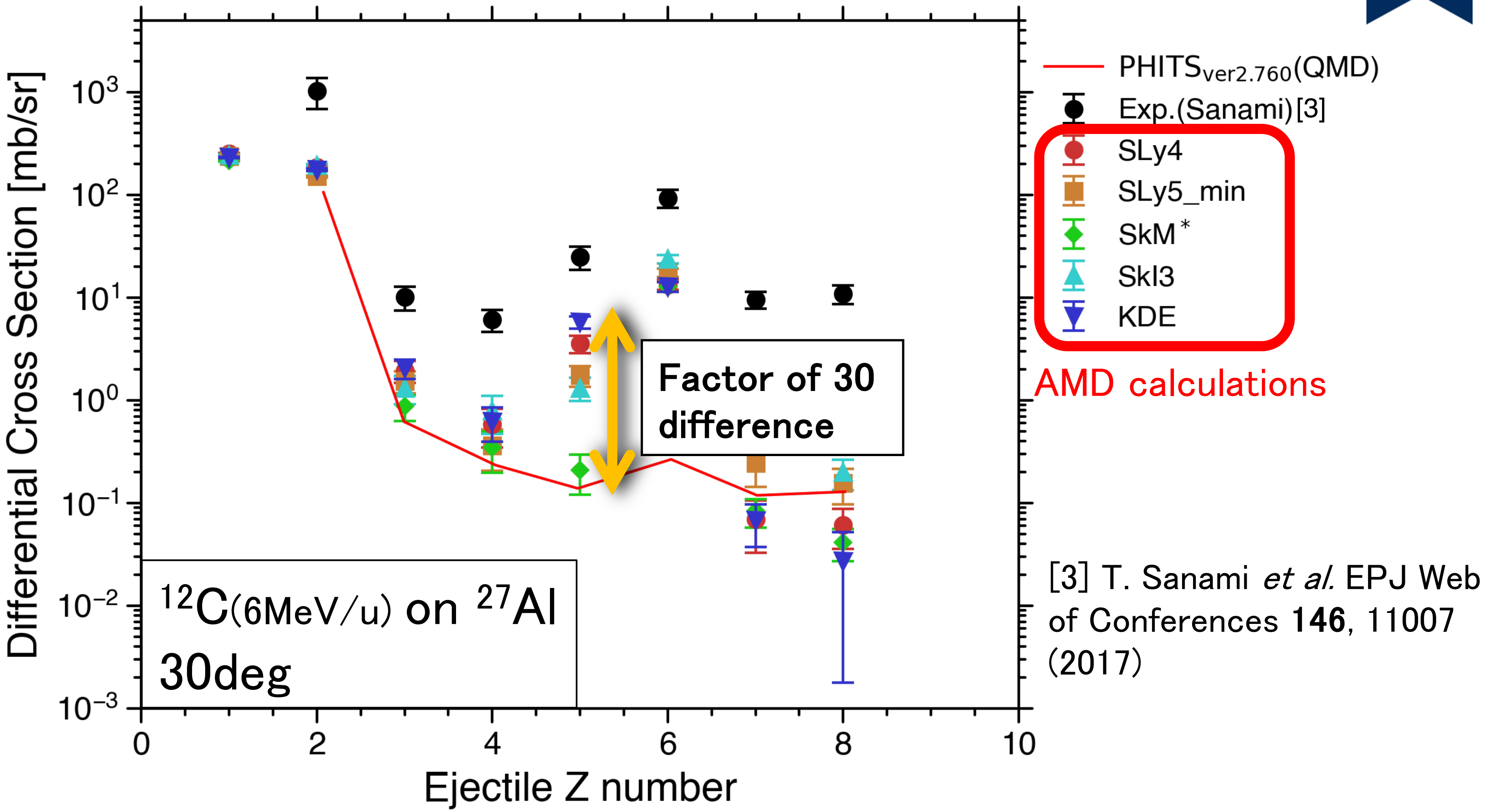
AMD, experimental values and PHITS



[3] T. Sanami *et al.* EPJ Web of Conferences **146**, 11007 (2017)

- Overall, PHITS data are underestimated compared to experimental data.
- The Z=6 bump structure is also underestimated.

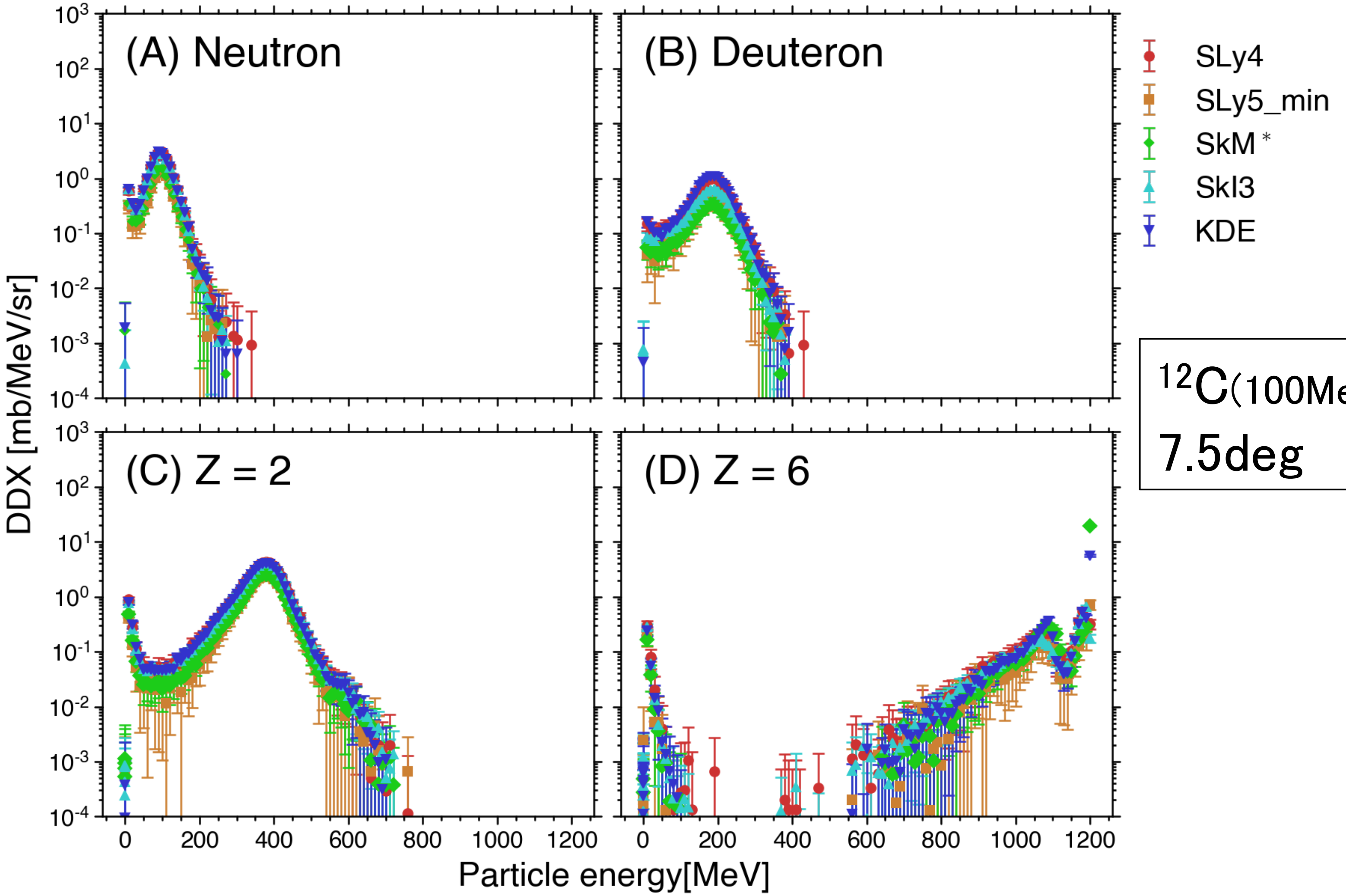
AMD, experimental values and PHITS



[3] T. Sanami *et al.* EPJ Web of Conferences **146**, 11007 (2017)

- The results for Z = 7 and 8 are not necessarily better than PHITS, but for Z = 2 to 6 they are better than PHITS.
- AMD reproduces the structure of the experimental data well.
- Overall, data reproducibility is equal to or better than PHITS.
- There is still a problem of underestimation overall.

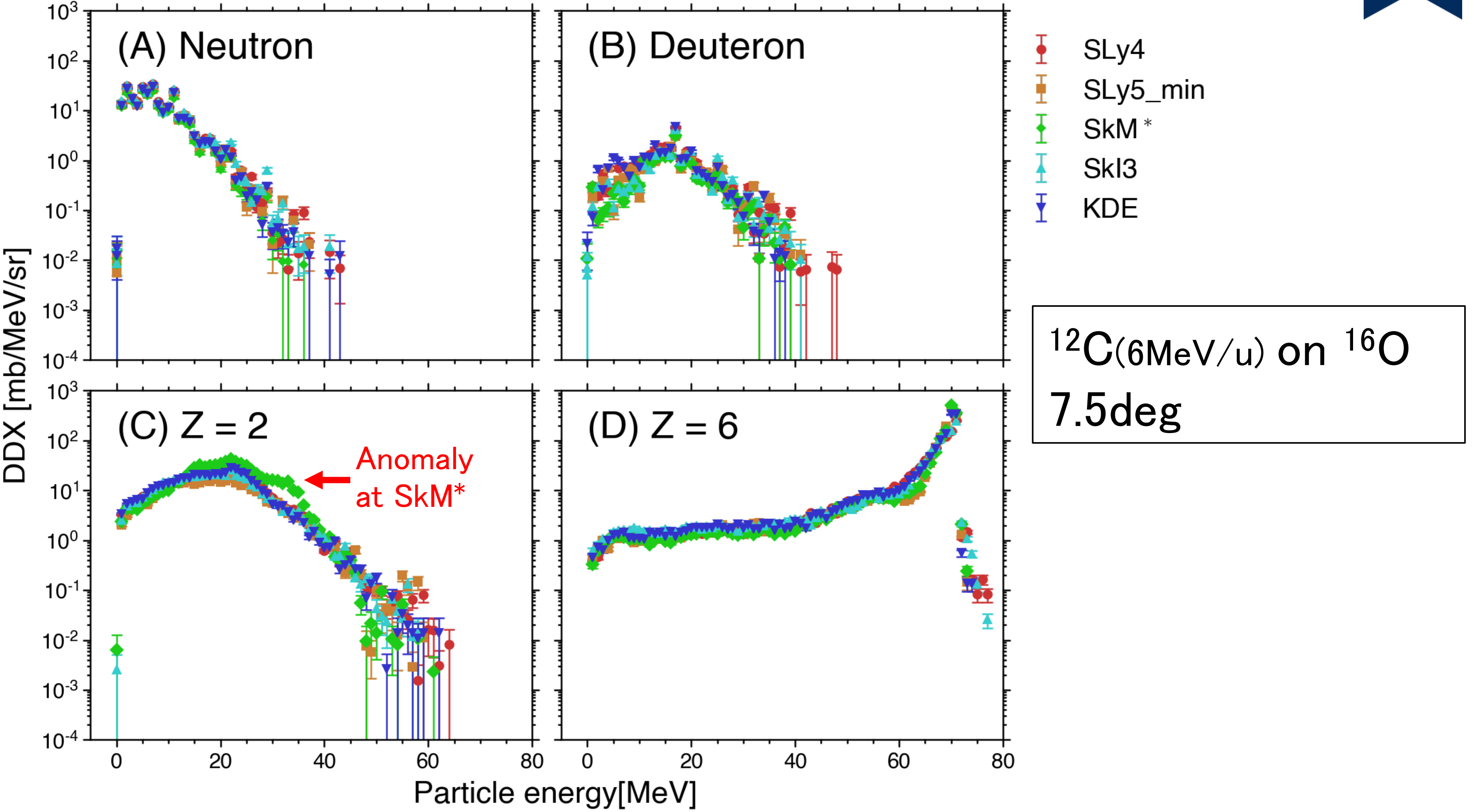
Comparison by DDX (2)



^{12}C(100MeV/u) on ^{16}O
7.5deg

- It can be seen that the distributions of each effective interaction have the same trend in all panels.
- Mean field effects are smaller for neutrons and Z=2 than for ^{27}Al targets.

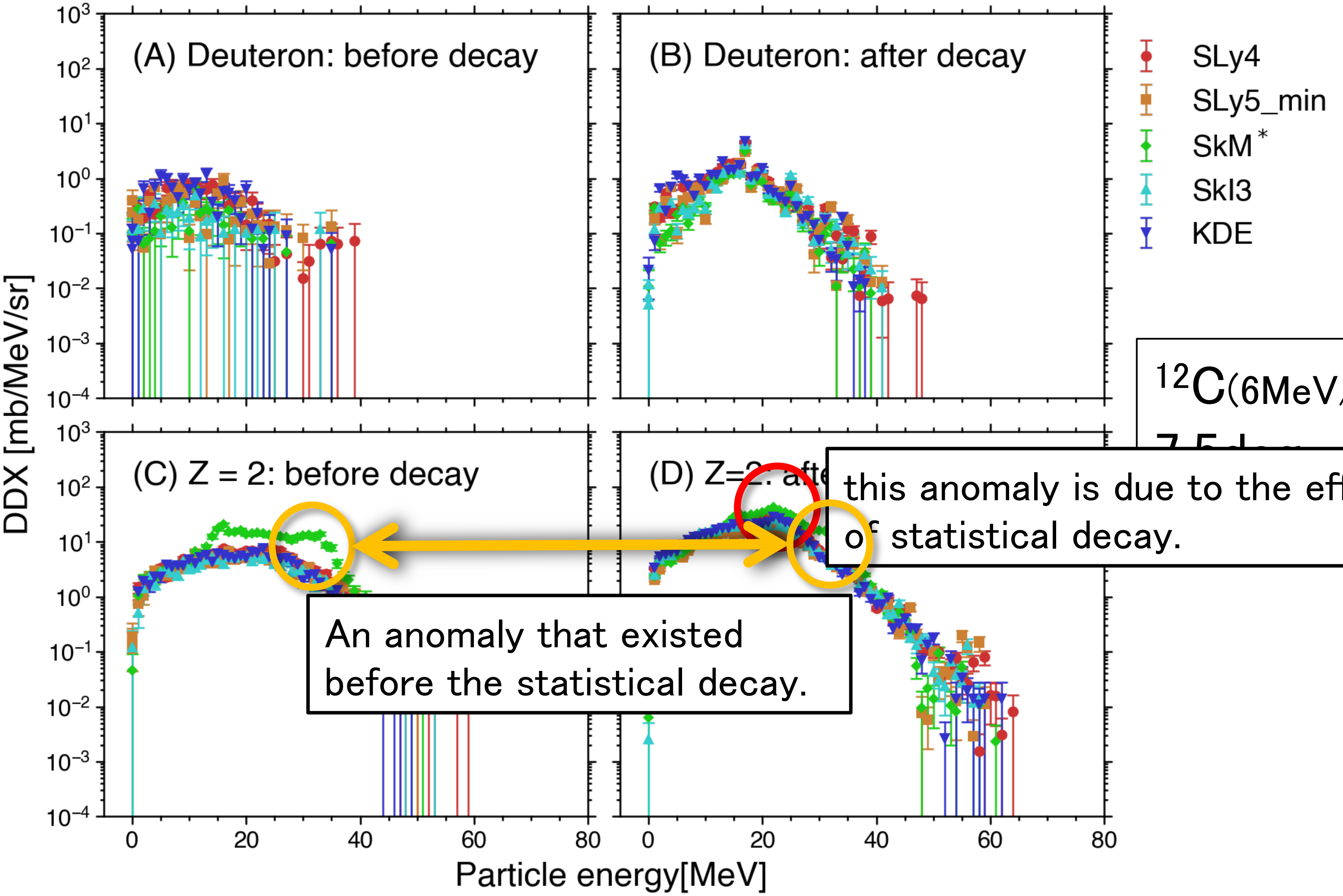
Comparison by DDX (3)



^{12}C(6MeV/u) on ^{16}O
7.5deg

- The mean-field effects of neutron and deuterons almost disappear.
- The helium isotopes differ in cross sections around 15–40 MeV.
- The carbon isotopes, there was the influence of the mean field around 60 MeV.
- The result at SkM* is particularly anomalous.

Comparison before and after statistical decay



^{12}C(6MeV/u) on ^{16}O
7.5deg

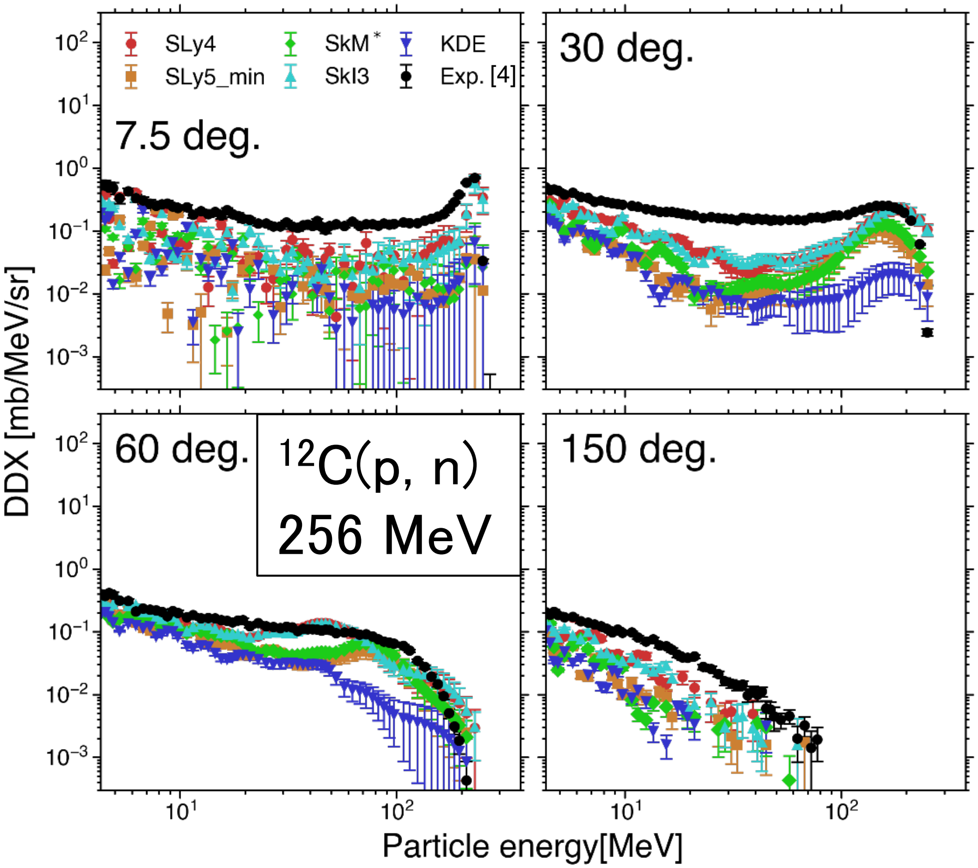
this anomaly is due to the effect of statistical decay.

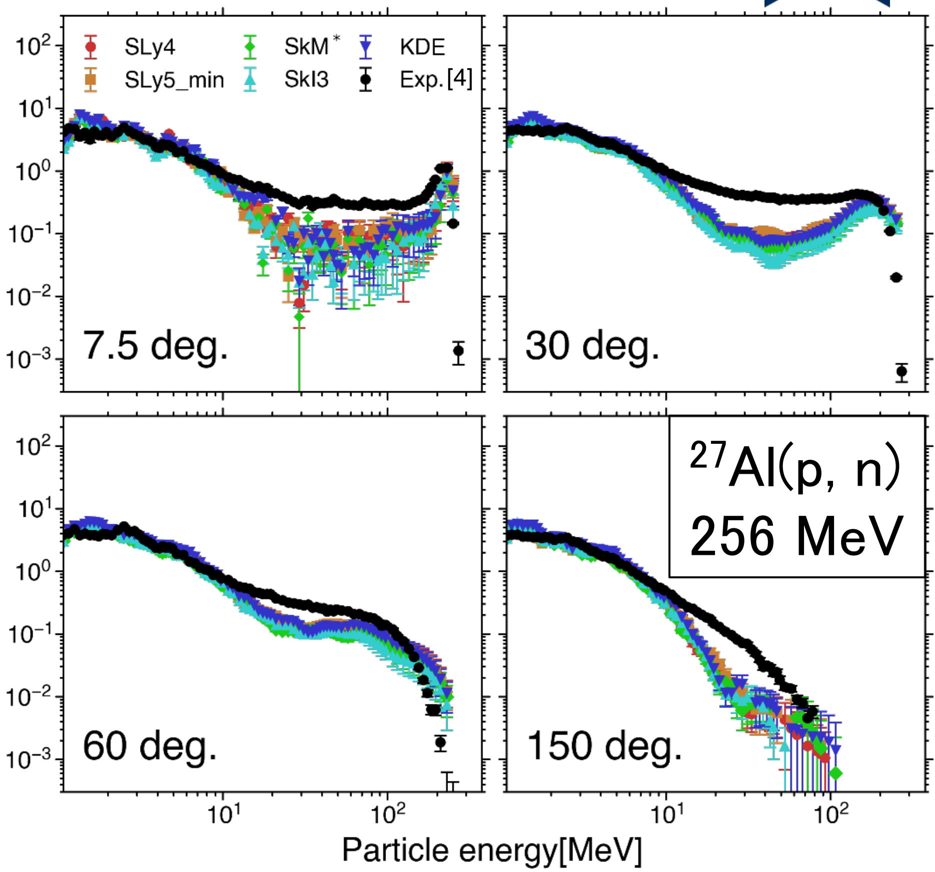
An anomaly that existed before the statistical decay.

In deuterons, the shape of the cross section changes significantly before and after statistical decay: results before the stat. decay reflects nuclear structure.

The effect of the mean field varies from nuclide to nuclide, but it is possible that the structure before statistical decay remains after the statistical decay, as in Z=2.

Comparison of ^{12}C(p, n) and ^{27}Al(p, n)





In all panels, the ^{12}C target is larger than the ^{27}Al. On the other hand, no mean–field effects are seen in the ^{27}Al cross section.

- This result is attributed to the fact that ^{12}C tends to form clusters, which leads to the complexity of the numerical calculations.
- It is thought that the way the ground state is described affects the cross section.

[4] M. M. Meier *et al.* Nucl. Sci. Eng. **110**, 289 (1992)

Summary

Nuclear reactions are used in astrophysics and medical field, so accurate evaluation is necessary.

→ AMD calculations were performed using 5 different effective interactions.

1. AMD does not always produce better results than PHITS.
2. The uncertainty increases with the cross-section of the forward emitted particles.
3. The mean-field effect is most likely influences cross sections of ^{12}C-induced reactions.
   → We believe this is because the ground state of ^{12}C tends to be a clustered structure.

Future issue

1. Investigate the effect of different reaction systems.
2. Systematize the effect of the mean field.