

FUS++ on Heavy-Ion Fusion Far Below the Barrier

Study on deep sub-barrier fusions within the improved coupled-channels method and Bayesian method

Peiwei Wen

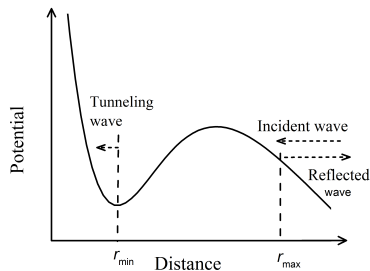
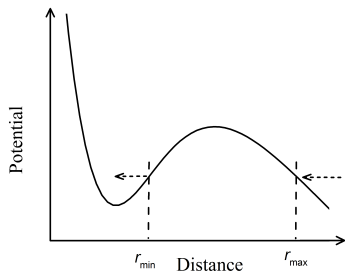
January 21, 2022



- 1 Introduction on deep sub-barrier fusions
- 2 The improved CC: CCFULL-FEM
- 3 Bayesian analysis on carbon fusion
- 4 Summary

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Time independent sub-barrier quantum tunneling



There are generally two ways to get the tunneling probability:

- Semi-classical approaches: WKB *et al.*

$$P_l^{\text{WKB}}(E) = \exp\left[-2 \int_{r_{\min}}^{r_{\max}} \sqrt{2\mu[V_l(r) - E]}/\hbar^2 dr\right],$$

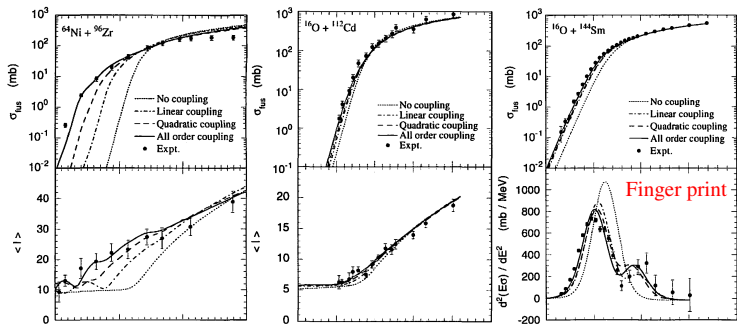
- Schrödinger equation under certain boundary conditions.

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} - E\right] \psi(r) = 0$$

Multi-channels problem for heavy-ion reactions

Taking into full order coupling in V_{nm} is important

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} + \epsilon_n - E \right] \psi_n(r) + \sum_m V_{nm}(r) \psi_m(r) = 0$$



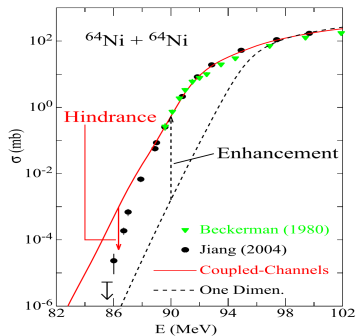
In CCFULL model, the full order couplings are considered.

H. Hagino *et al*, PRC. 55, 276 (1997).
 M. Dasgupta *et al*, Annu. Rev. Nucl. Part. S 48, 401 (1998);
 H. Hagino *et al*, Comput. Phys. Commun. 123 143 (1999);

Discovery of deep sub-barrier fusion hindrance

B. B. Back, H. Esbensen, C. L. Jiang and K. E. Rehm (2014). *Rev. Mod. Phys.* 86: 317.

"The comparison with CC calculations using a Woods-Saxon potential allowed them to cleanly identify the fusion hindrance at the lowest energies."



C. L. Jiang, B. B. Back, et al. (2021), *Eur. Phys. J. A*, 57, 235.

Argonne National Laboratory Experiments:

C. L. Jiang, H. Esbensen et al,
Phys Rev Lett 89 (5), 052701 (2002);
Phys Rev Lett 93 (1), 012701 (2004);
Phys Rev Lett 113 (2), 022701 (2014).

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ANU Experiments:

M. Dasgupta, D. J. Hinde, A. Diaz-Torres, et al,
Phys Rev Lett 99, 192701 (2007).

.....

INFN Experiments:

G. Montagnoli, A. M. Stefanini, et al,
Physics Letters B 728: 639. (2014)
Physical Review C 97(2): 024610.(2018)
Physical Review C 100(4): 044619. (2019).

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Mumbai Experiments:

Shrivastava, A., et al,
Phys Rev C, 96, 034620 (2017);
Phys Rev Lett, 103, 232702. (2009)

.....

Deep sub-barrier fusion hindrance & S factor

PHYSICAL REVIEW C **97**, 012801(R) (2018)

Rapid Communications

Reaction rate for carbon burning in massive stars

C. L. Jiang,¹ D. Santiago-Gonzalez,^{1,2} S. Almaraz-Calderon,^{1,3} K. E. Rehm,¹ B. B. Back,¹ K. Auranen,¹ M. L. Avila,¹

Carbon burning is a critical phase for nucleosynthesis in massive stars. The conditions for igniting this burning stage, and the subsequent isotope composition of the resulting ashes, depend strongly on the reaction rate for $^{12}\text{C} + ^{12}\text{C}$ fusion at very low energies. Results for the cross sections for this reaction are influenced by various backgrounds encountered in measurements at such energies. In this paper, we report on a new measurement of $^{12}\text{C} + ^{12}\text{C}$ fusion cross sections where these backgrounds have been minimized. It is found that the astrophysical S factor exhibits a maximum around $E_{\text{cm}} = 3.5\text{--}4.0$ MeV, which leads to a reduction of the previously predicted astrophysical reaction rate.

PRL **113**, 022701 (2014)

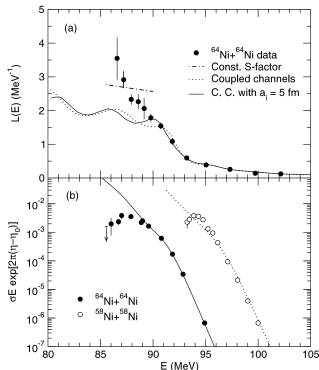
PHYSICAL REVIEW LETTERS

week ending
11 JULY 2014

Fusion Hindrance for a Positive- Q -Value System $^{24}\text{Mg} + ^{30}\text{Si}$

C. L. Jiang,^{1,7} A. M. Stefanini,² H. Esbensen,¹ K. E. Rehm,¹ S. Almaraz-Calderon,¹ B. B. Back,¹ L. Corradi,² E. Fioretto,² G. Montagnoli,³ F. Scarlassara,³ D. Montanari,³ S. Courtin,⁴ D. Bourgin,⁴ F. Haas,⁴ A. Goussuff,⁵ S. Szilner,⁶ and T. Mijatovic⁶

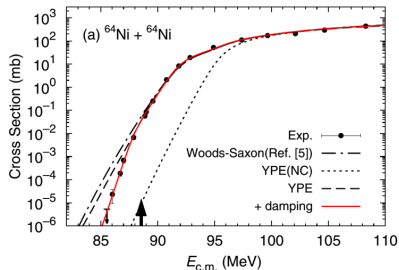
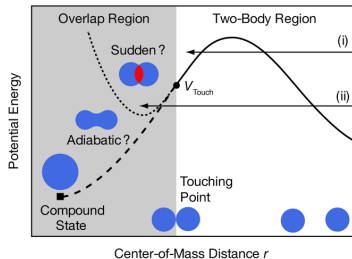
Measurements of the excitation function for the fusion of $^{24}\text{Mg} + ^{30}\text{Si}$ ($Q = 17.89$ MeV) have been extended toward lower energies with respect to previous experimental data. The S-factor maximum observed in this large, positive- Q -value system is the most pronounced among such systems studied thus far. The significance and the systematics of an S-factor maximum in systems with positive fusion Q values are discussed. This result would strongly impact the extrapolated cross sections and reaction rates in the carbon and oxygen burnings and, thus, the study of the history of stellar evolution.



$$\langle \sigma v \rangle \approx \left(\frac{2}{\mu}\right)^{\frac{1}{2}} \frac{\Delta E_0}{(kT)^{3/2}} S(E_0) \exp\left(-\frac{3E_0}{kT}\right); \quad S(E) = \sigma E \exp(2\pi\eta); \quad \eta = \frac{Z_1 Z_2 e^2}{4\pi \epsilon_0 \hbar v}$$

Fusion between light nuclei is of interest because its important roles in the late stages of massive star evolution.

Explanations: adiabatic approximation & deep potential

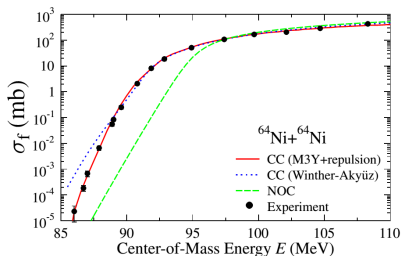
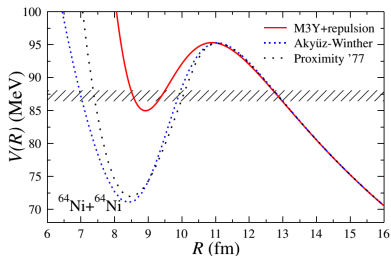


- T. Ichikawa, K. Hagino and A. Iwamoto, Phys Rev C 75, 064612 (2007); Phys Rev Lett 103, 202701 (2009); T. Ichikawa, Phys Rev C 92 (6), 064604 (2015).

On top of the conventional CC method, an extra one-dimensional adiabatic potential barrier is assumed after the reacting nuclei contact with each other, considering the formation of the composite system.

- K. Hagino, A. B. Balantekin, N. W. Lwin et al, Phys Rev C 97, 034623 (2018).
Two Woods-Saxon potentials with different slopes.

Explanations: sudden approximation & shallow potential



- Ş. Mişicu and H. Esbensen, Phys Rev Lett 96 (11), 112701 (2006); Phys Rev C 75, 034606 (2007);

Hindrance of Heavy-Ion Fusion due to Nuclear Incompressibility. Double-folding potential with M3Y forces supplemented by a repulsive core.

- C. Simenel, A. S. Umar, K. Godbey, et al, Phys Rev C 95, R031601 (2017).

Density constrained time dependent Hartree-Fock model. It is concluded that: " ...to explain experimental fusion data at deep sub-barrier energies, then cannot be justified by an effect of incompressibility. It is more likely that it simulates other effects such as Pauli repulsion."

- V. V. Sargsyan, G. G. Adamian, N. V. Antonenko et al, Eur Phys J A 56, 19 (2020).

Extended quantum diffusion approach + Double folding potential.

About deep sub-barrier fusion hindrance:

- Whether could the CC calculation of the fusion cross section be stable at the deep sub-barrier energy region?

Some works used an extra imaginary potential around the potential minimum to eliminate the fluctuations of the conventional CC calculation. However, one has to add more parameters.

- Is Woods-Saxon potential able to describe the deep sub-barrier fusion hindrance phenomenon well enough?

It is said that it is not able to describe it in many works. And hybrid potential model, other potential models, and reaction mechanisms are widely used now.

- What's the mechanism of the fusion hindrance?

The shallow potential or deep potential.

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Import gradients for solving the coupled-channels equation

There are several parts to construct the coupled-channels approach:

① Nuclear potential:

real potential (double folding, proximity, **Woods-Saxon potential**), complex potential

② Coupled potential:

full order coupling, linear coupling, or the quadratic coupling

③ Boundary condition:

regular boundary condition, **incoming wave boundary condition**

④ Numerical method:

finite difference method (Numerov , three-point difference), finite element method (**KANTBP**), R-matrix method.

O. Chuluunbaatar, A. A. Gusev, *et al*, CPC. 177, 649 (2007)

A. A. Gusev, O. Chuluunbaatar, S. I. Vinitisky *et al*, CPC 185, 3341 (2014)

The incoming wave boundary condition

The incoming wave boundary conditions (IWBC)

$$\psi_n(r) = \begin{cases} T_n \exp(-ik_n(r_{\min})r), & r \leq r_{\min} \\ H_l^-(k_n r) \delta_{n,0} + R_n H_l^+(k_n r), & r \geq r_{\max} \end{cases}$$

Here $k_n = k_n(r \rightarrow +\infty)$, and $k_n(r)$ is the local wave number for n -th channel

$$k_n(r) = \sqrt{\frac{2\mu}{\hbar^2} \left(E - \epsilon_n - \frac{l(l+1)\hbar^2}{2\mu r^2} - V_N^{(0)}(r) - \frac{Z_P Z_T e^2}{r} - V_{nn}(r) \right)}$$

There are problems in the previous boundary condition.

- The plane wave boundary condition at the left boundary r_{\min} involves only the diagonal part. This requires that the off-diagonal matrix elements tend to zero.
- However, at r_{\min} , the distance between two nuclei is so short that the off-diagonal matrix elements are usually not zero. There can be sudden noncontinuous changes in the left boundary.
- A linear transformation should be done at the left boundary.

V.V. Samarin, V.I. Zagrebaev, 2004 *NPA* **734** E9;

V.I. Zagrebaev, V.V. Samarin, 2004 *Phys. Atom. Nucl.* **67** 1462;

The new method KANTBP

The coupled-channels Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} + \epsilon_n - E \right] \psi_{nm_o} + \sum_{n'=1}^N V_{nn'}(r) \psi_{n'n_o}(r) = 0, \quad (1)$$

with

- n_o is a number of the open entrance channel with a positive relative energy $E_{n_o} = E - \epsilon_{n_o} > 0, n_o = 1, \dots, N_o \leq N$.
- $\{\psi_{nm_o}(r)\}_{n=1}^N$ are components of a desirable matrix solution.

Let \mathbf{W} is the symmetric matrix of dimension $N \times N$

$$W_{nm} = W_{mn} = \frac{2\mu}{\hbar^2} \left[\left(\frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} + \epsilon_n \right) \delta_{nm} + V_{nm}(r) \right]. \quad (2)$$

Then the equation can be expressed as

$$-\psi_{nm}''(r) + \sum_{m'} W_{nm'} \psi_{m'm}(r) = \frac{2\mu E}{\hbar^2} \psi_{nm}(r), \quad (3)$$

The new method KANTBP

Diagonalize the matrix at $r = r_{\min}$

$$\mathbf{WA} = \mathbf{A}\tilde{\mathbf{W}}, \quad \{\tilde{\mathbf{W}}\}_{nm} = \delta_{nm}\tilde{W}_{mm}, \quad \tilde{W}_{11} \leq \tilde{W}_{22} \dots \leq \tilde{W}_{NN}. \quad (4)$$

The functions $y_m(r)$ are solutions of the uncoupled equations

$$y_m''(r) + K_m^2 y_m(r) = 0, \quad K_m^2 = \frac{2\mu E}{\hbar^2} - \tilde{W}_{mm}. \quad (5)$$

In open channels at $K_m^2 > 0$, $m = 1, \dots, M_o \leq N$ the solutions $y_m(r)$ have the form:

$$y_m(r) = \frac{\exp(-\imath K_m r)}{\sqrt{K_m}}. \quad (6)$$

In this case $\psi_{m_o}(r)$ expressed by the linear combinations of the linear independent solutions

$$\psi_{m_o}(r) = \sum_{m=1}^{M_o} A_{nm} y_m(r) \hat{T}_{m_n o}, \quad r = r_{\min}. \quad (7)$$

In this way, the off-diagonal matrix elements have been considered in the calculation.

The new method KANTBP

Summary of the boundary conditions for open channels

$$\psi_{n_n o}^{as}(r) = \begin{cases} \sum_{m=1}^{M_o} A_{nm} \frac{\exp(-\nu K_m r)}{\sqrt{K_m}} \hat{T}_{mn_o}, & r = r_{\min}, \\ \hat{H}_l^-(k_n r) \delta_{n,n_o} + \hat{H}_l^+(k_n r) \hat{R}_{mn_o}, & r = r_{\max}. \end{cases} \quad (8)$$

In this case the partial tunneling probability from the ground state ($n_o = 1$) is

$$P_l(E) \equiv T_{n_o n_o}^{(l)}(E). \quad (9)$$

At fixed orbital momentum l , it is given by summation over all possible intrinsic states:

$$T_{n_o n_o}^{(l)}(E) = \sum_{m=1}^{M_o} |\hat{T}_{mn_o}|^2, \quad R_{n_o n_o}^{(l)}(E) = \sum_{n=1}^{N_o} |\hat{R}_{nn_o}|^2, \quad T_{n_o n_o}^{(l)}(E) = 1 - R_{n_o n_o}^{(l)}(E) \quad (10)$$

The condition $T_{n_o n_o}^{(l)}(E) + R_{n_o n_o}^{(l)}(E) - 1 = 0$ fulfills with ten significant digits by the element method KANTBP.

O. Chuluunbaatar, A. A. Gusev, A.G. Abrashkevich *et al*, CPC. 177, 649 (2007)

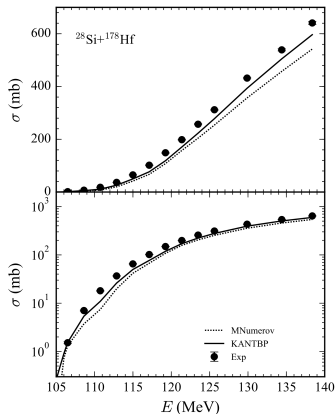
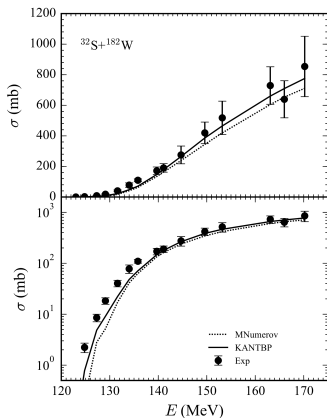
A. A. Gusev, O. Chuluunbaatar, S. I. Vinitsky *et al*, CPC 185, 3341 (2014)

A. A. Gusev, O. Chuluunbaatar, S. I. Vinitsky *et al*, Math. Mod. Geom. 3, 2 22 (2015)

V. I. Zagrebaev, Phys. Rev. C 78 047602 (2008)

$^{32}\text{S}+^{182}\text{W}$, $^{28}\text{Si}+^{178}\text{Hf}$: Near barrier fusion

S. I. Vinitzky, P. W. Wen, A. A. Gusev, O. Chuluunbaatar, R. G. Nazmitdinov, A. K. Nasirov, C. J. Lin, H. M. Jia and A. Gózdź, Acta Phys. Pol. B Proc. Suppl. 13 (3), 549 (2020).



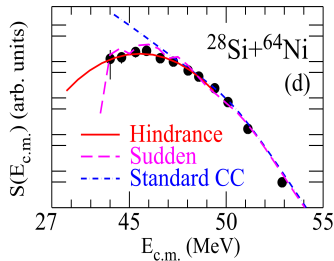
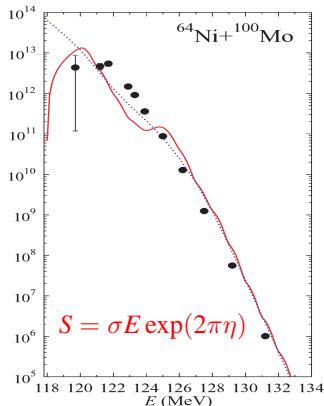
There are obvious differences in sub-barrier energy region.

Hindrance of Heavy-Ion Fusion due to Nuclear Incompressibility

Ş. Mişicu* and H. Esbensen

Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

(Received 26 January 2006; published 21 March 2006)



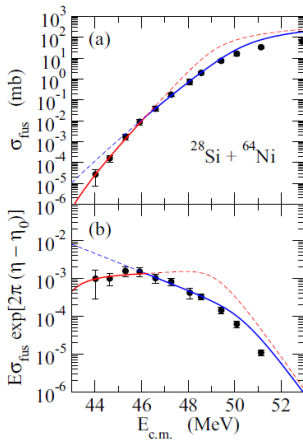
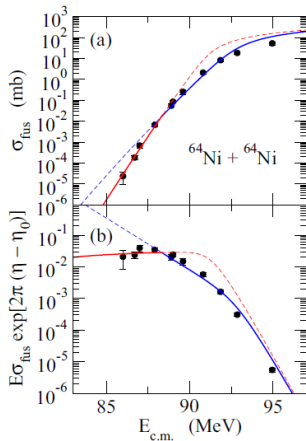
The M3Y+repulsion potential is usually used.

$^{64}\text{Ni} + ^{100}\text{Mo}$, $^{28}\text{Si} + ^{64}\text{Ni}$: Deep sub-barrier fusion

Two potentials including a larger (smaller) logarithmic slope at energies lower (higher) than the threshold energy

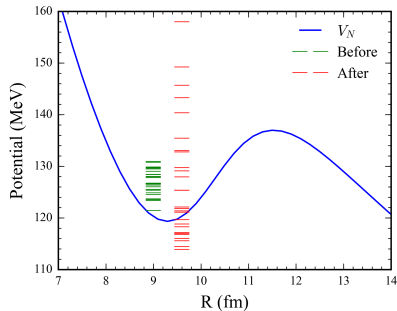
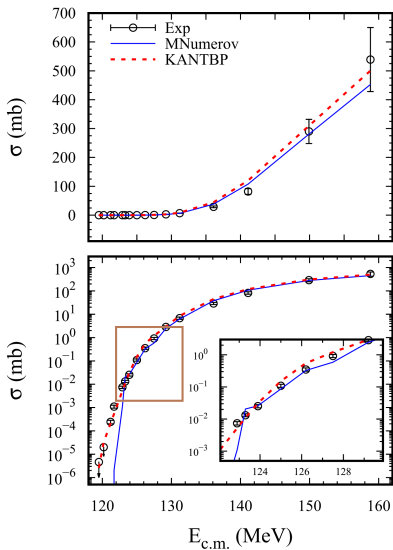
HAGINO, BALANTEKIN, LWIN, AND THEIN

PHYSICAL REVIEW C 97, 034623 (2018)



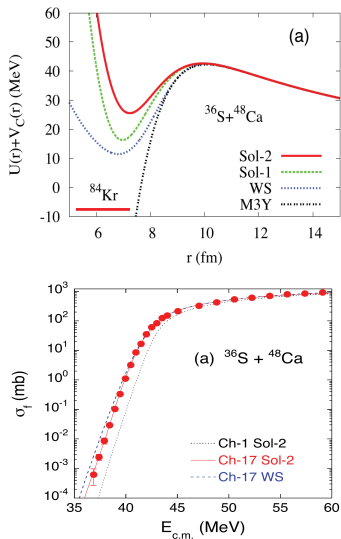
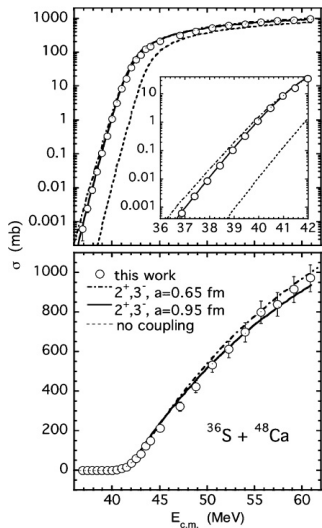
$^{64}\text{Ni} + ^{100}\text{Mo}$: Deep sub-barrier fusion

P.W. Wen, O. Chuluunbaatar, A.A. Gusev, et al. (2020). Phys Rev C 101, 014618.



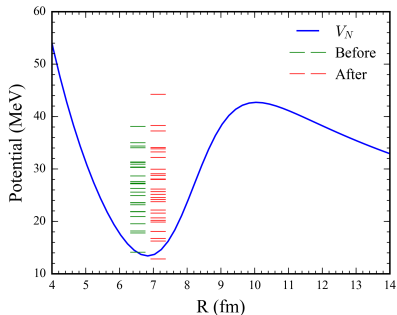
New calculations are more stable
and agree with experimental data
better

$^{36}\text{S}+^{48}\text{Ca}$: Deep sub-barrier fusion



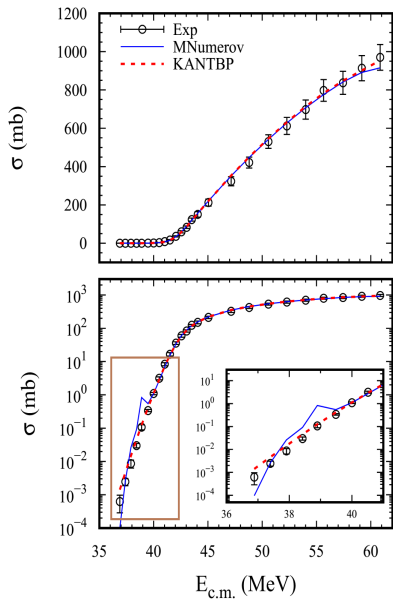
The M3Y+repulsion potential is usually used. The weak imaginary potential is adopted to eliminate some unwanted fluctuations.

$^{36}\text{S} + ^{48}\text{Ca}$: Deep sub-barrier fusion



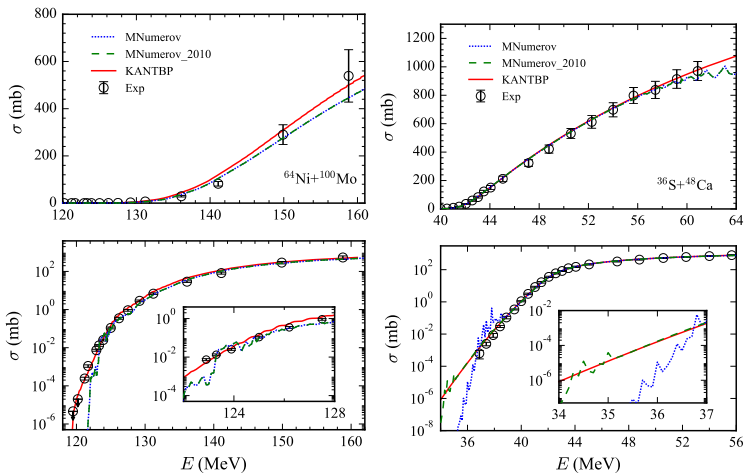
New calculations are more stable,
and are higher than experimental
data at deep sub-barrier energy.

P. W. Wen, O. Chuluunbaatar, et al, *Phys. Rev. C*,
101:014618, 2020.



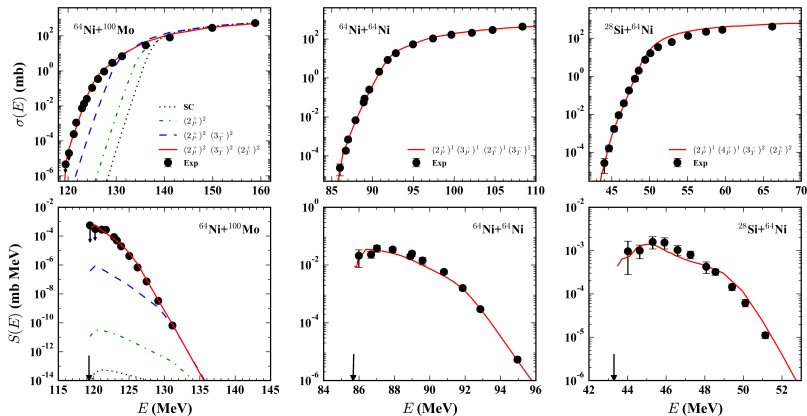
A strict test with $\Delta E = 0.1$ MeV (preliminary)

Chuluunbaatar O, Gusev AA, Vinitsky SI, Abrashkevich AG, Wen PW, Lin CJ. Submitted to Computer Physics Communications. (KANTBP3.1 & CCFULL-FEM)



There are obvious differences in both sub-barrier and above-barrier energy regions.

P. W. Wen, C. J. Lin, R. Nazmitdinov, S. I. Vinitys, et al. *PRC*, 103, 054601, 2021.

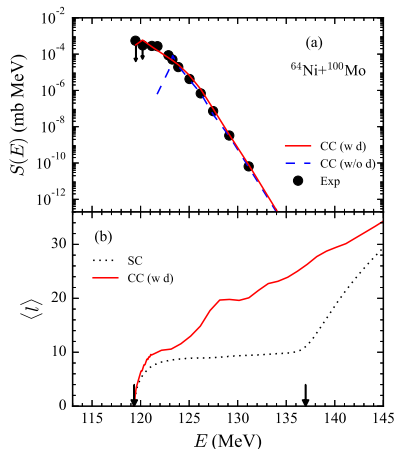
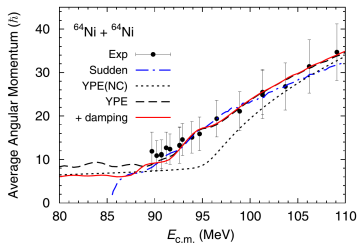


Woods-Saxon potential and multiphonon coupling are enough.

$^{64}\text{Ni} + ^{100}\text{Mo}$: Potential details

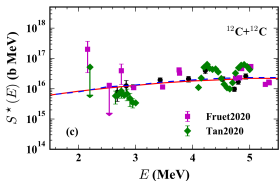
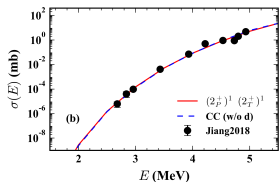
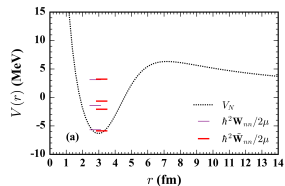
TABLE I. Woods-Saxon potential parameters V_0 (MeV), a_0 (fm), and R_0 (fm) for $^{64}\text{Ni} + ^{100}\text{Mo}$, $^{64}\text{Ni} + ^{64}\text{Ni}$, and $^{28}\text{Si} + ^{64}\text{Ni}$ reaction systems. The potential barrier V_B and the minimum of the potential pocket V_P are also listed.

	$^{64}\text{Ni} + ^{100}\text{Mo}$	$^{64}\text{Ni} + ^{64}\text{Ni}$	$^{28}\text{Si} + ^{64}\text{Ni}$
V_0 (MeV)	79.938	65.829	53.529
a_0 (fm)	0.686	0.801	0.944
R_0 (fm)	10.190	9.239	7.790
V_B (MeV)	136.993	96.389	51.946
V_P (MeV)	119.344	85.699	43.298

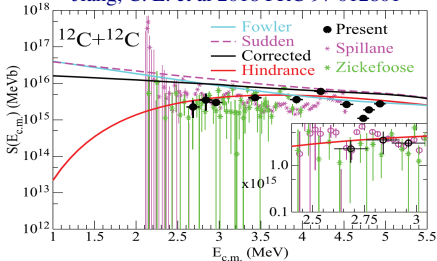


$\langle l \rangle$ could be used as a probe to separate these two mechanisms.

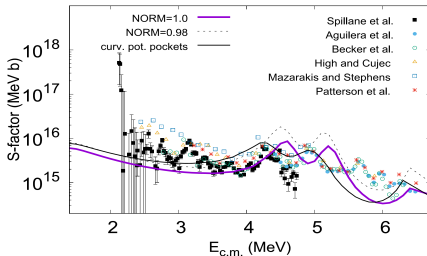
Ichikawa, T. Phys Rev C 92, 064604 (2015).



Jiang, C. L. et al 2018 PRC 97 012801



A. Diaz-Torres, et al, 2018 PRC 97 055802



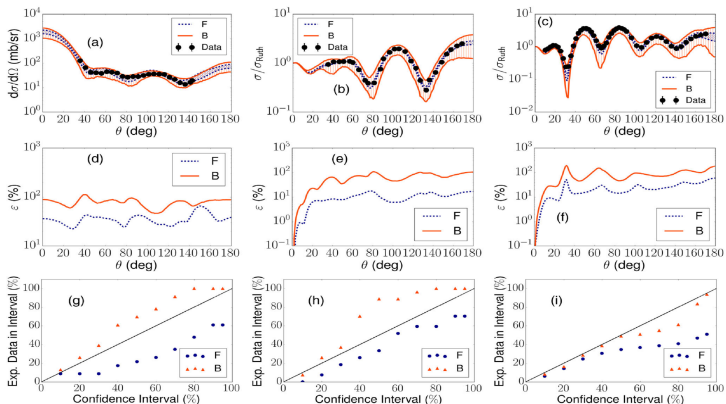
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Bayesian method vs Frequentist method

PHYSICAL REVIEW LETTERS **122**, 232502 (2019)

Direct Comparison between Bayesian and Frequentist Uncertainty Quantification for Nuclear Reactions

G. B. King,^{1,2} A. E. Lovell,^{3,4} L. Neufcourt,^{1,5} and F. M. Nunes^{1,2,*}



$^{48}\text{Ca}(n,n)$ 12 MeV

$^{48}\text{Ca}(p,p)$ 14 MeV

$^{48}\text{Ca}(p,p)$ 25 MeV

Bayesian method: more flexible, represent reality more accurately

Bayesian method

The posterior probability distribution functions:

$$P(x | D) = \frac{P(D | x)P(x)}{P(D)}$$

- $P(x)$: uniform prior distribution of the model parameter x .

Yang, L., Lin, C. J., Zhang, Y. X., Wen, P. W., et al. (2020) Phys. Lett. B 807, 135540

"We found that the ... parameters strongly depends on the prior knowledge ... We suggest that... a flat distribution could be employed as a convincing prior knowledge of the Bayesian framework. "

- $P(D | x)$: the likelihood function with a Gaussian distribution. $P(D)$ is the normalization constant and integrates to 1.

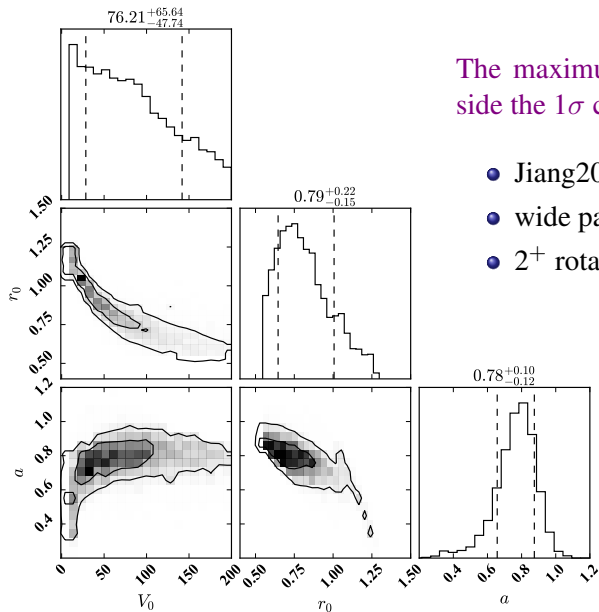
The Markov chain Monte Carlo algorithm *emcee*:

- The sampling depends on a few tuning parameters.
- It uses an ensemble of walkers which can be moved in parallel.

D. Foreman-Mackey, D. W. Hogg, D. Lang, et al. Publ Astron Soc Pac 125, 306 (2013).

D. P. Fleming, R. Barnes, R. Luger, and J. T. VanderPlas, Astrophys J 891, 155 (2020).

Test results (preliminary)

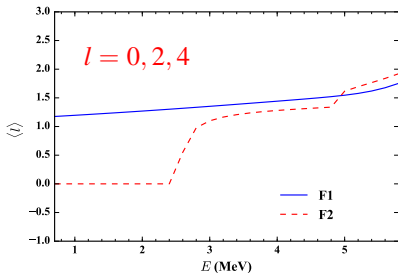
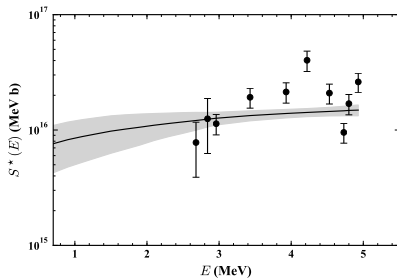
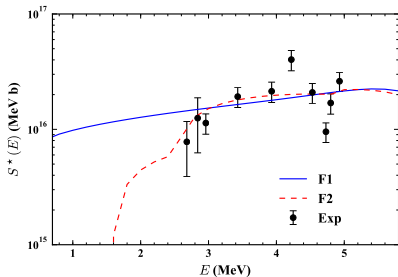


The maximum peak of V_0 is outside the 1 σ confidence interval.

- Jiang2018 experimental data.
- wide parameter range
- 2⁺ rotation coupling

Bayesian method vs MIGRAD in Minuit (preliminary)

James, F., Roos, M. (1975). Comput. Phys. Commun., 10(6), 343-367.

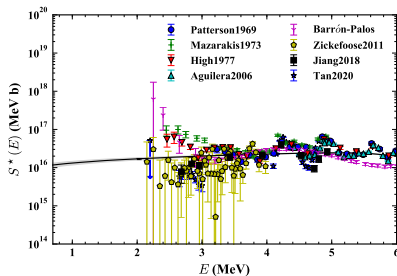
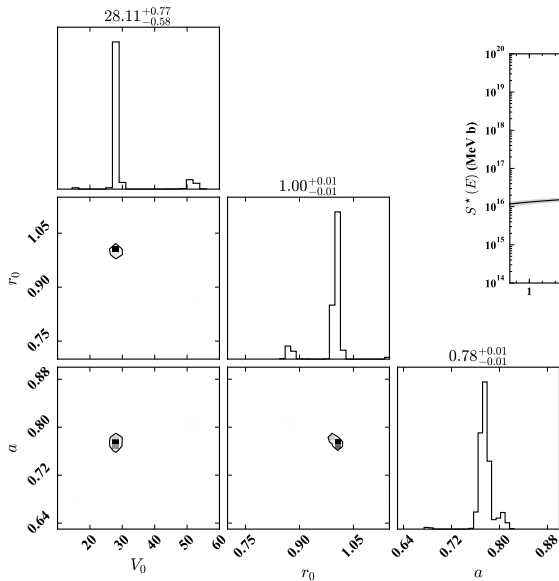


- F1: $V_0 = 59.67^{+32.14}$ MeV, $a = 0.91^{+0.30}$ fm, $r_0 = 0.76^{+0.17}$ fm
- F2: $V_0 = 13.05^{+0.51}$ MeV, $a = 0.69^{+0.02}$ fm, $r_0 = 1.16^{+0.01}$ fm

The search based on the MIGRAD method is easily trapped in the local minimums near the initial value.

More experimental data (preliminary)

T. P. Luo, P. W. Wen, C.J. Lin, Lei, Yang et al. submitted to Chin. Phys. C



Narrow distributions

No obvious maximum

- 1 Introduction on deep sub-barrier fusions
- 2 The improved CC: CCFULL-FEM
- 3 Bayesian analysis on carbon fusion
- 4 Summary

- The **CCFULL-FEM** approach with **KANTBP3.1** could reproduce the **the deep sub-barrier fusion cross sections**, as well as the **S factor**, of several typical reactions by using the most simple **WS potential** and multiphonon couplings.
- **The Bayesian method** is more powerful than the MIGRAD approach, and its analysis shows **no hindrance for $^{12}\text{C}+^{12}\text{C}$ fusion reaction** between 1 ~ 3 MeV (preliminary).
- $\langle I \rangle$ could be used to clarify the mechanism of shallow or deep potential, especially for **$^{12}\text{C}+^{12}\text{C}$** reaction.

Chuluunbaatar O, Gusev AA, Vinitzky SI, Abrashkevich AG, Wen PW, Lin CJ. Submitted to Computer Physics Communications. (KANTBP3.1 & CCFULL-FEM)

Thank my collaborators of these works:

- China Institute of Atomic energy, Beijing

Chengjian Lin, Huiming Jia, Lei Yang, Tianpeng Luo, Feng Yang,
et al

- Joint Institute of Nuclear Physics, Dubna

S. I. Vinitsky, O. Chuluunbaatar, R. Nazmitdinov, G. G. Gusev,
A. Nasirov, et al

Thank you for your attention !