Describing low-energy nuclear reactions with quantum wave-packet dynamics

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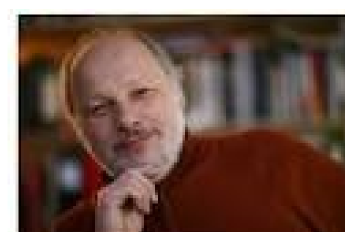
UNIVERSITY OF SURREY

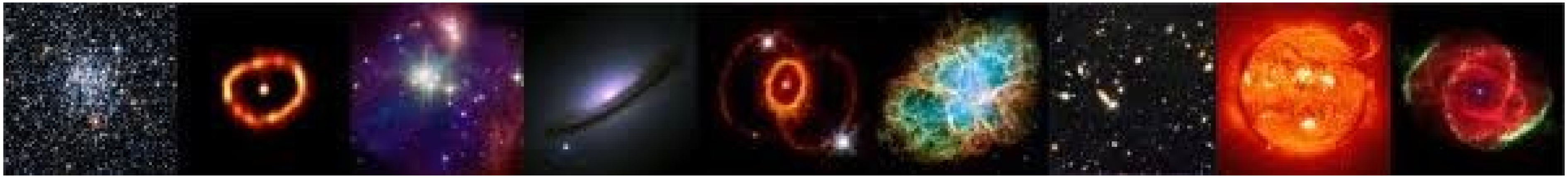
Examples

- $^{6}Li + {}^{209}Bi$

- $^{12}C + {}^{12}C$



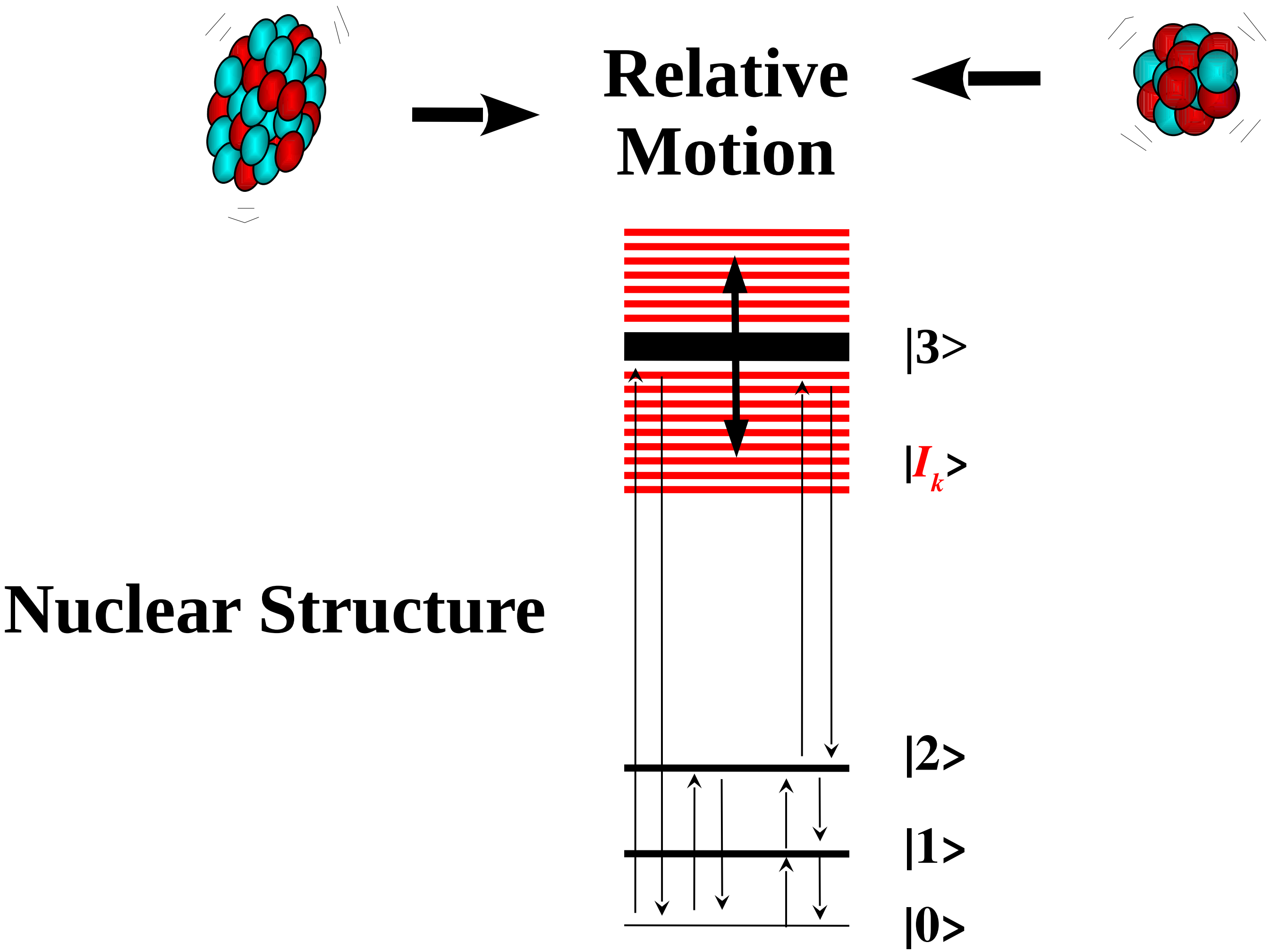
Importance of the Physics of Nuclear Reactions



- **This physics** is crucial for understanding **energy production** and **element creation** in the Universe.

- **Nuclear reactions** are the **primary probe** of the **New Physics**.

The Physics of Low-Energy Nuclear Reactions



Interplay between **nuclear structure** and **reaction dynamics** determines reaction outcomes (**cross sections**)

Quantum Wave-Packet Dynamics

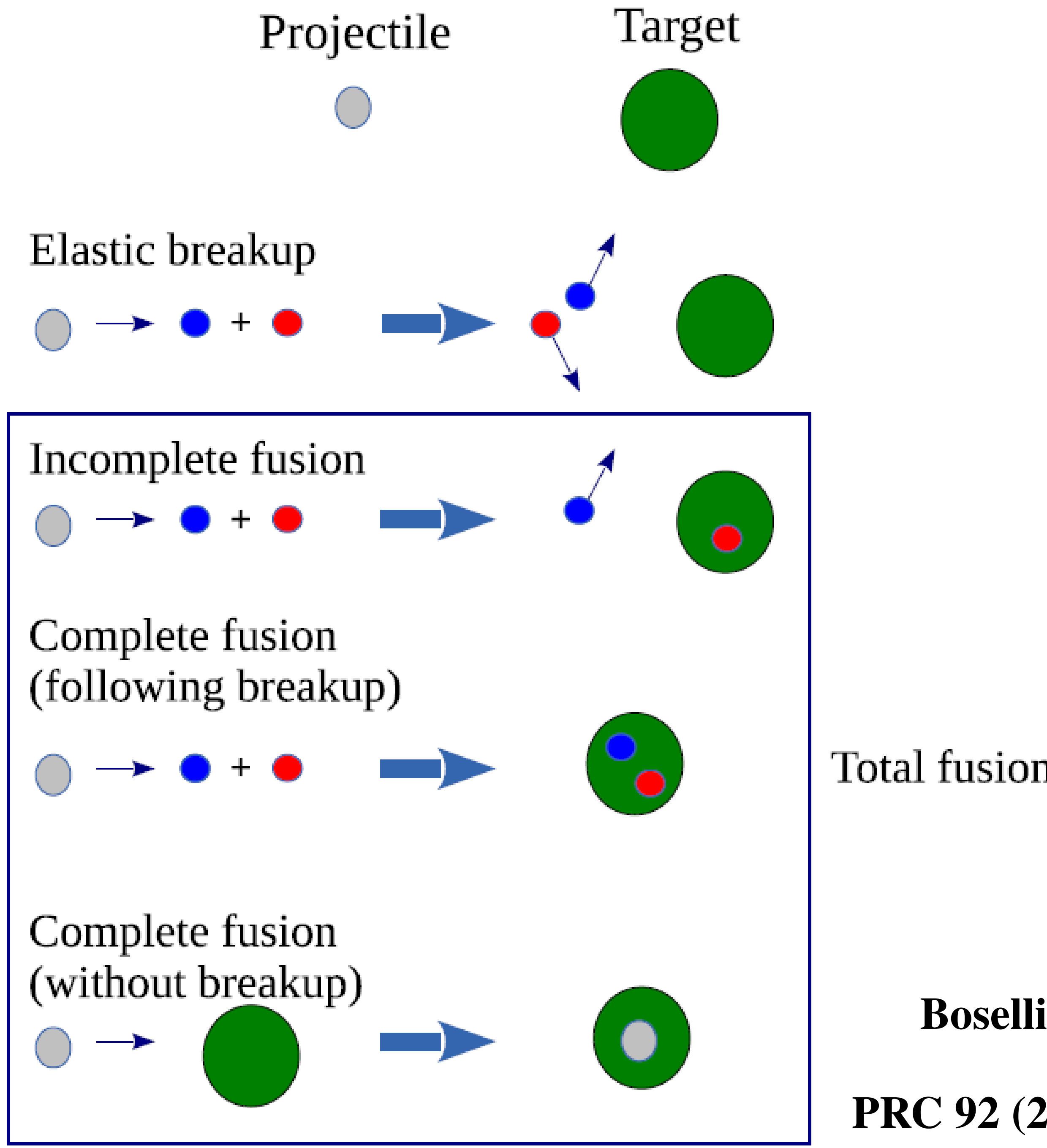
D.J. Tannor, Quantum Mechanics: a Time-Dependent Perspective, USB, 2007

- **Preparation:** the initial state $\Psi(t=0)$

- **Time propagation:** $\Psi(0) \longrightarrow \Psi(t)$,
  guided by the operator, $\exp(-i\,\hat{H}\,t/\hbar)$
  $\hat{H}$ is the model Hamiltonian

- **Analysis:** extraction of probabilities from the time-dependent wave function

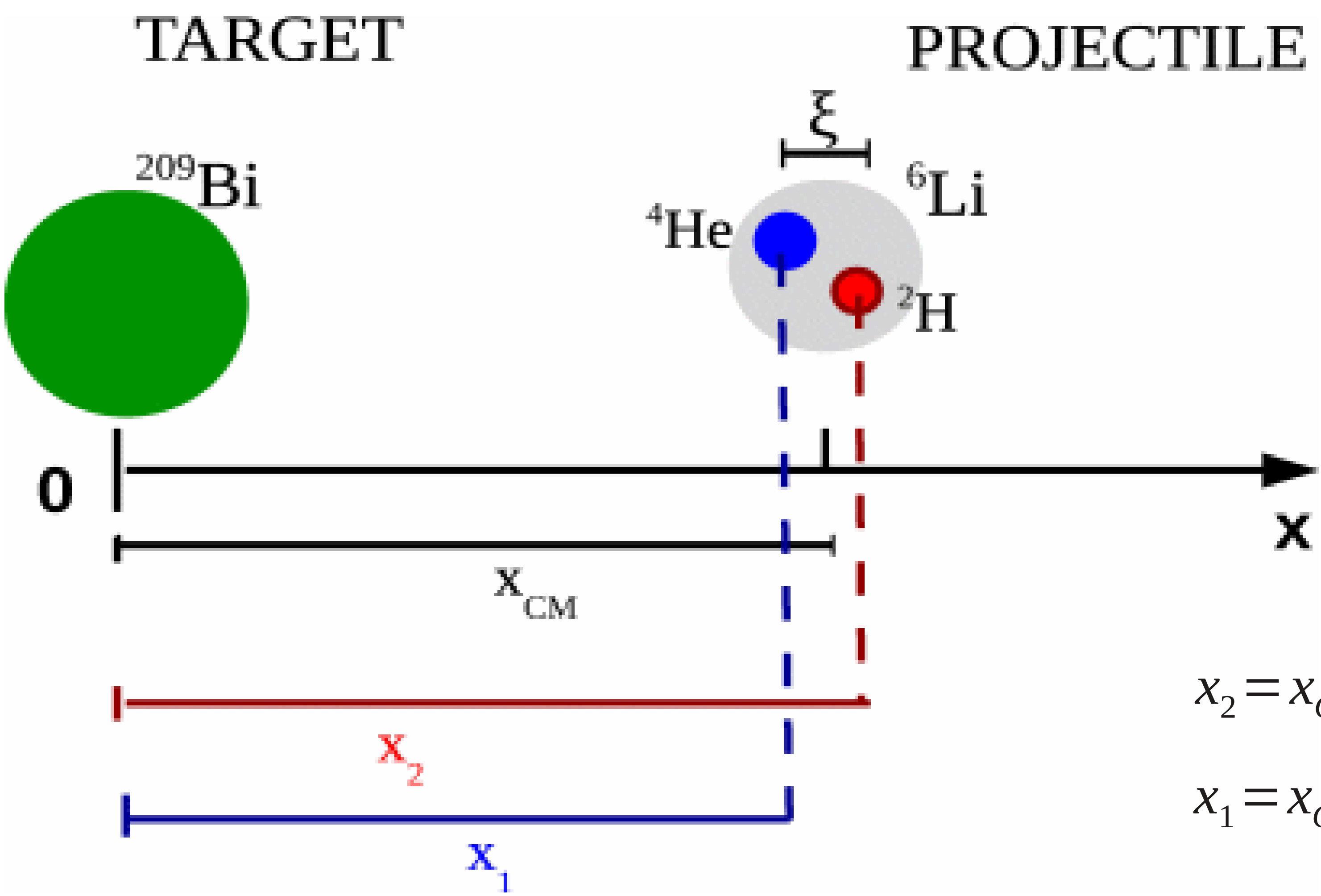
Fusion Dynamics of Weakly Bound Nuclei



Boselli & AD-T,

PRC 92 (2015) 0446110

One-Dimensional Toy Model



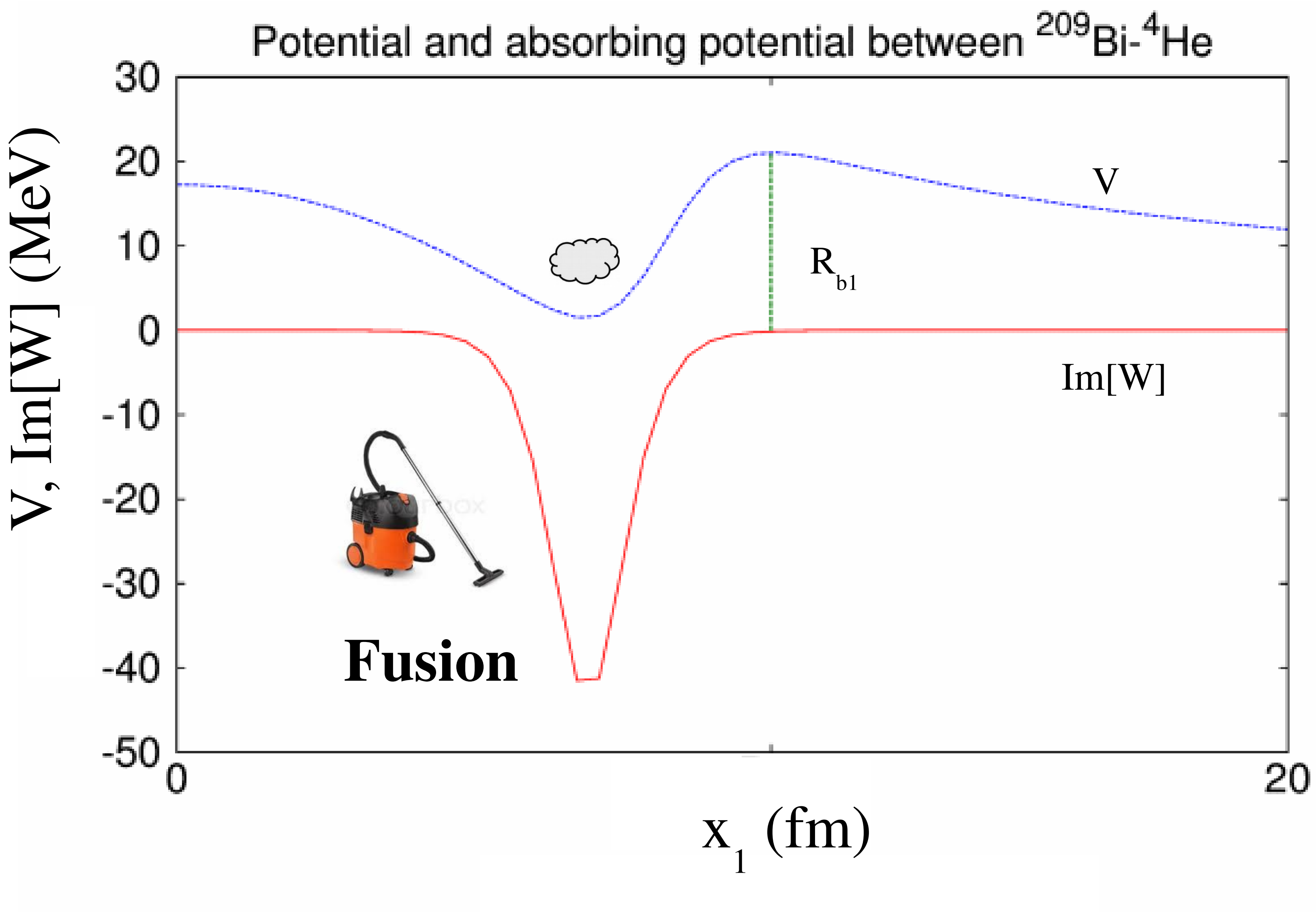
$$x_2 = x_{CM} + b\,\xi$$

$$x_1 = x_{CM} - a\,\xi$$

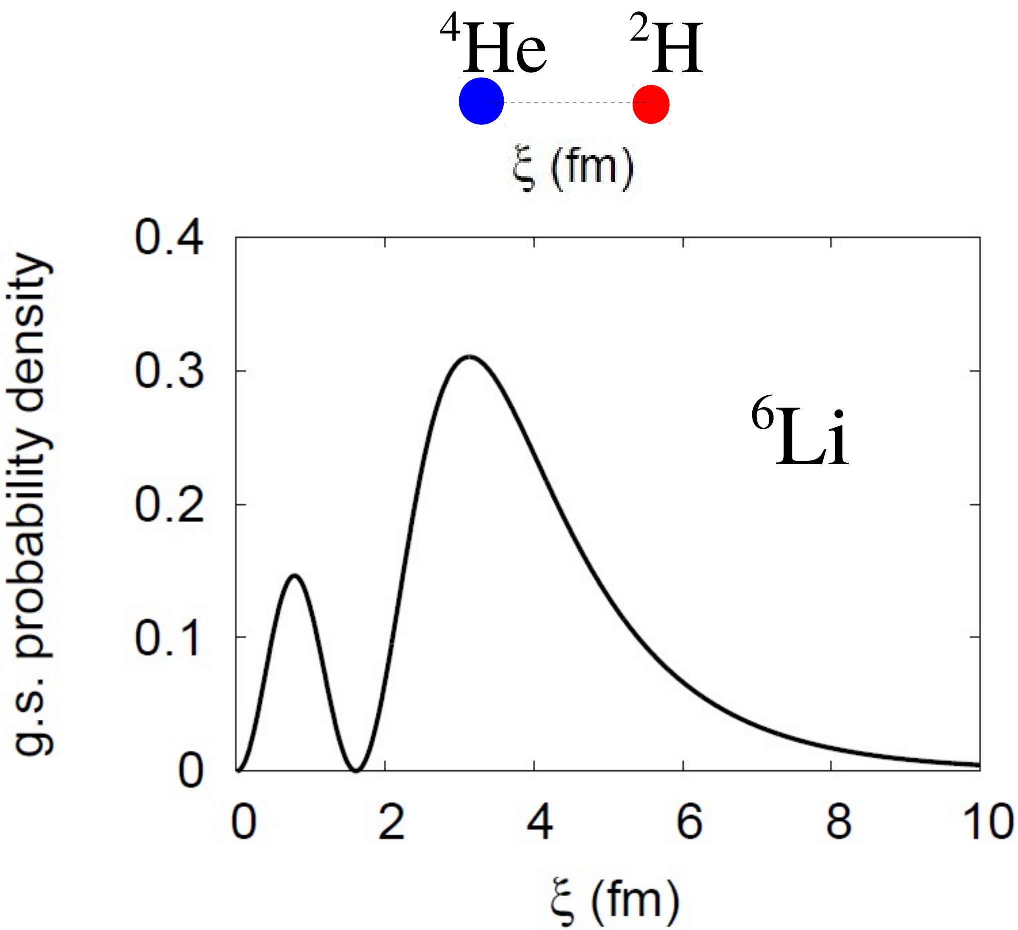
$$H = \frac{P_{x_{CM}}^2}{2\mathrm{M}_{T12}} + \frac{P_{\xi}^{\,2}}{2\mathrm{m}_{12}} + U_{12}(\xi) + V_{T1}(x_{CM} - a\,\xi) + V_{T2}(x_{CM} + b\,\xi)$$

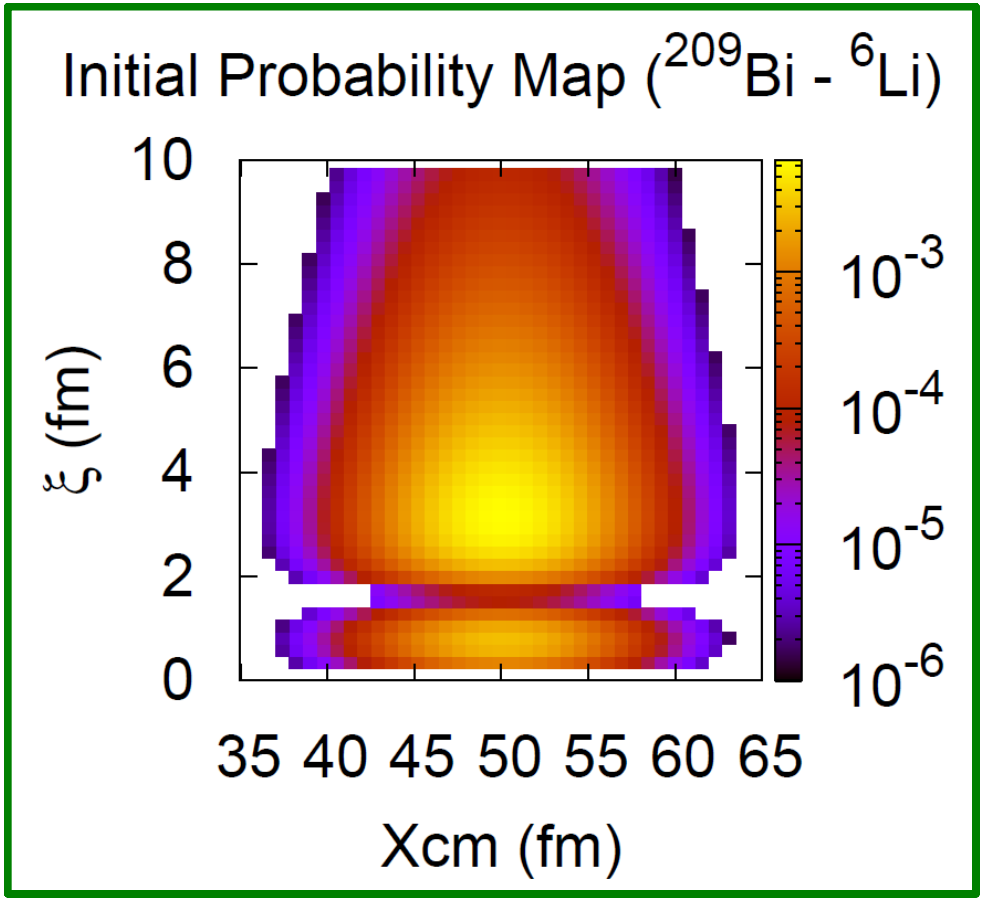
Describing Fusion

- To simulate fusion (**irreversibility**): acting inside the Coulomb barrier $\boxed{-iW_{T1}(x_1)}$ & $\boxed{-iW_{T2}(x_2)}$



Preparing the Initial State





Time Propagation

R. Kosloff, Ann. Rev. Phys. Chem. **45** (1994) 145

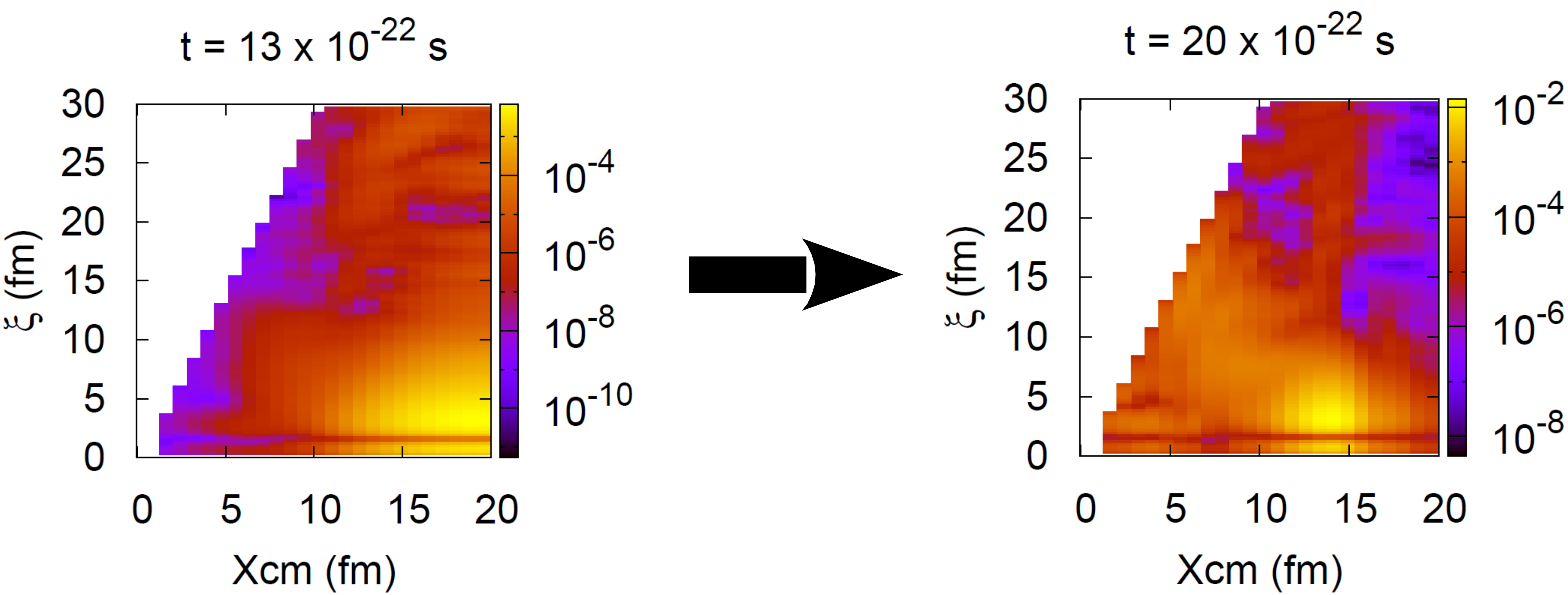
$$\Psi(t+\Delta t) = \exp\left(-i\frac{\hat{H}\,\Delta t}{\hbar}\right)\Psi(t)$$

$$\exp\left(-i\frac{\hat{H}\,\Delta t}{\hbar}\right) \approx \sum_n a_n\, Q_n(\hat{H}_{norm})$$

$$\hat{H}_{norm} = \frac{(\bar{H}\,\hat{1} - \hat{H})}{\Delta H}$$

The Chebyshev Propagator

$$a_n = i^n(2-\delta_{n0})\exp(-i\frac{\bar{H}\,\Delta t}{\hbar})\,J_n(\frac{\Delta H\,\Delta t}{\hbar})$$



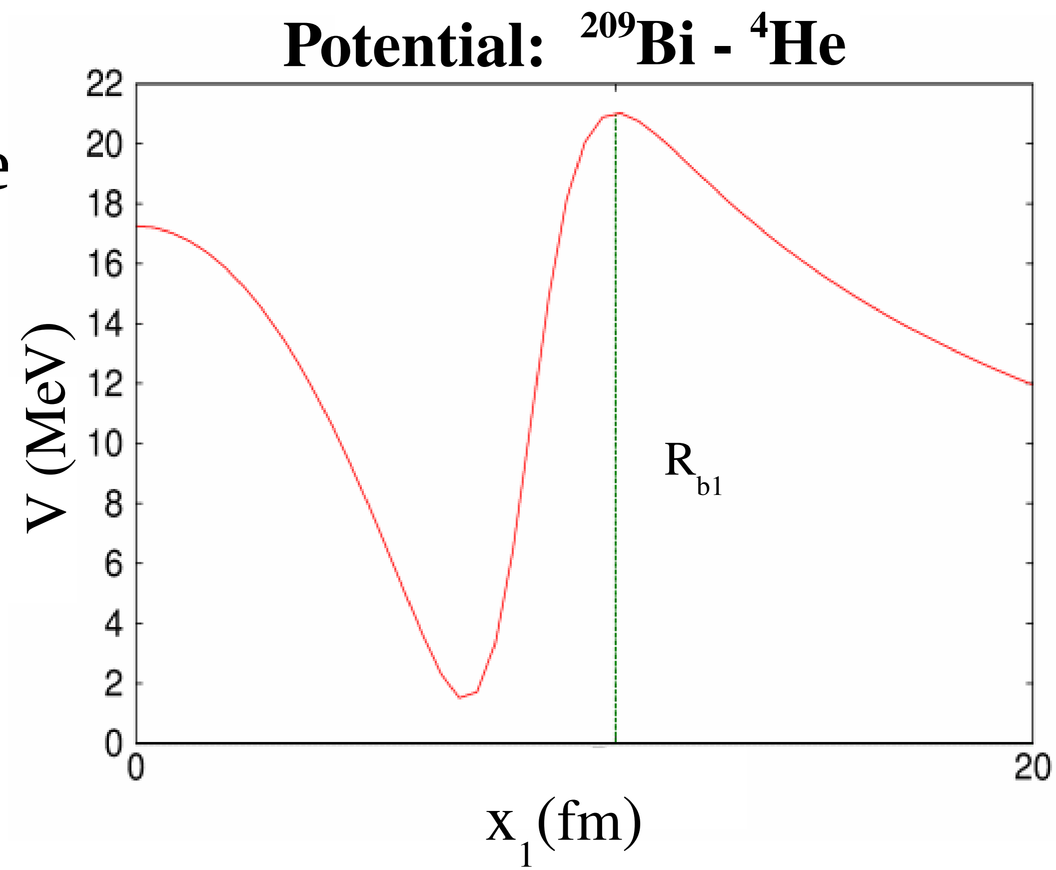
Analysis: Slicing the Wave Function

- Projection operator acting on the position x_i of the fragment relative to the target

(Heaviside function)

$$P_i = \Theta\left(R_{bi} - x_i\right)$$
$$Q_i = 1 - P_i$$

- Act with $\left(P_1 + Q_1\right)\left(P_2 + Q_2\right) = 1$ on the wave function:

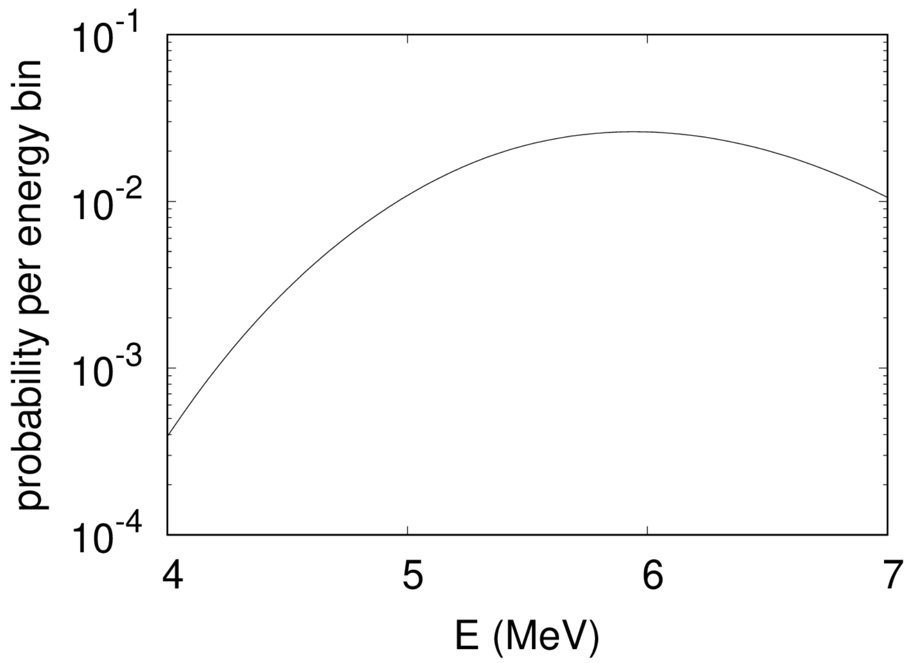


	CAPTURED	NON CAPTURED
CF	● ●	
ICF	●	●

$$\tilde{\Psi}\left(x_1, x_2, t\right) = \left(P_1 P_2 + P_1 Q_2 + Q_1 P_2 + Q_1 Q_2\right) \tilde{\Psi}\left(x_1, x_2, t\right) = \Psi_{CF} + \Psi_{ICF} + \Psi_{SCATT}$$

Energy Projection of the Wave Function

Schafer & Kulander,
PRA **42** (1990) 5794



- **Energy spectra** of $\Psi(t)$
  as expectation values
  of **the window operator**

$$\hat{\boldsymbol{\Delta}}(E_k, n, \epsilon) \equiv \frac{\epsilon^{2^n}}{(\hat{\mathcal{H}} - E_k)^{2^n} + \epsilon^{2^n}}$$

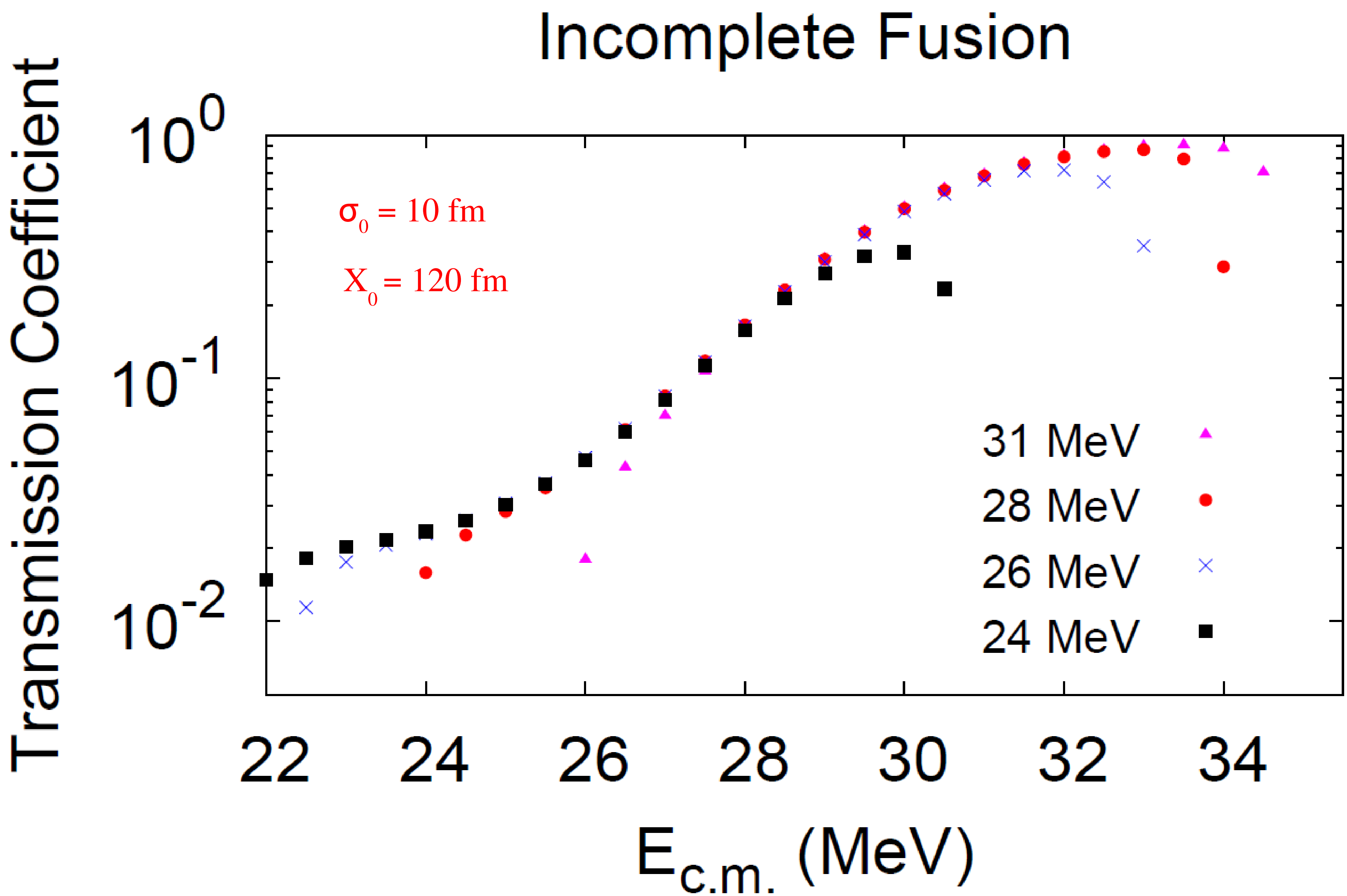
$$E_{k+1} = E_k + 2\epsilon$$

- $\mathcal{P}(E_k) = \langle\Psi|\hat{\Delta}|\Psi\rangle$, for instance, **n = 2** :

$$\boxed{(\hat{H} - E_k + \sqrt{i}\,\epsilon)(\hat{H} - E_k - \sqrt{i}\,\epsilon)\,|\chi_k\rangle = \epsilon^2\,|\Psi\rangle}$$

$$\rightarrow \quad \boxed{\mathcal{P}(E_k) = \langle\chi_k|\chi_k\rangle}$$

Results



Incomplete Fusion
Transmission Coefficient
10^0
10^{-1}
10^{-2}
σ_0 = 10 fm
X_0 = 120 fm
31 MeV
28 MeV
26 MeV
24 MeV
22
24
26
28
30
32
34
$E_{c.m.}$ (MeV)

Summarising

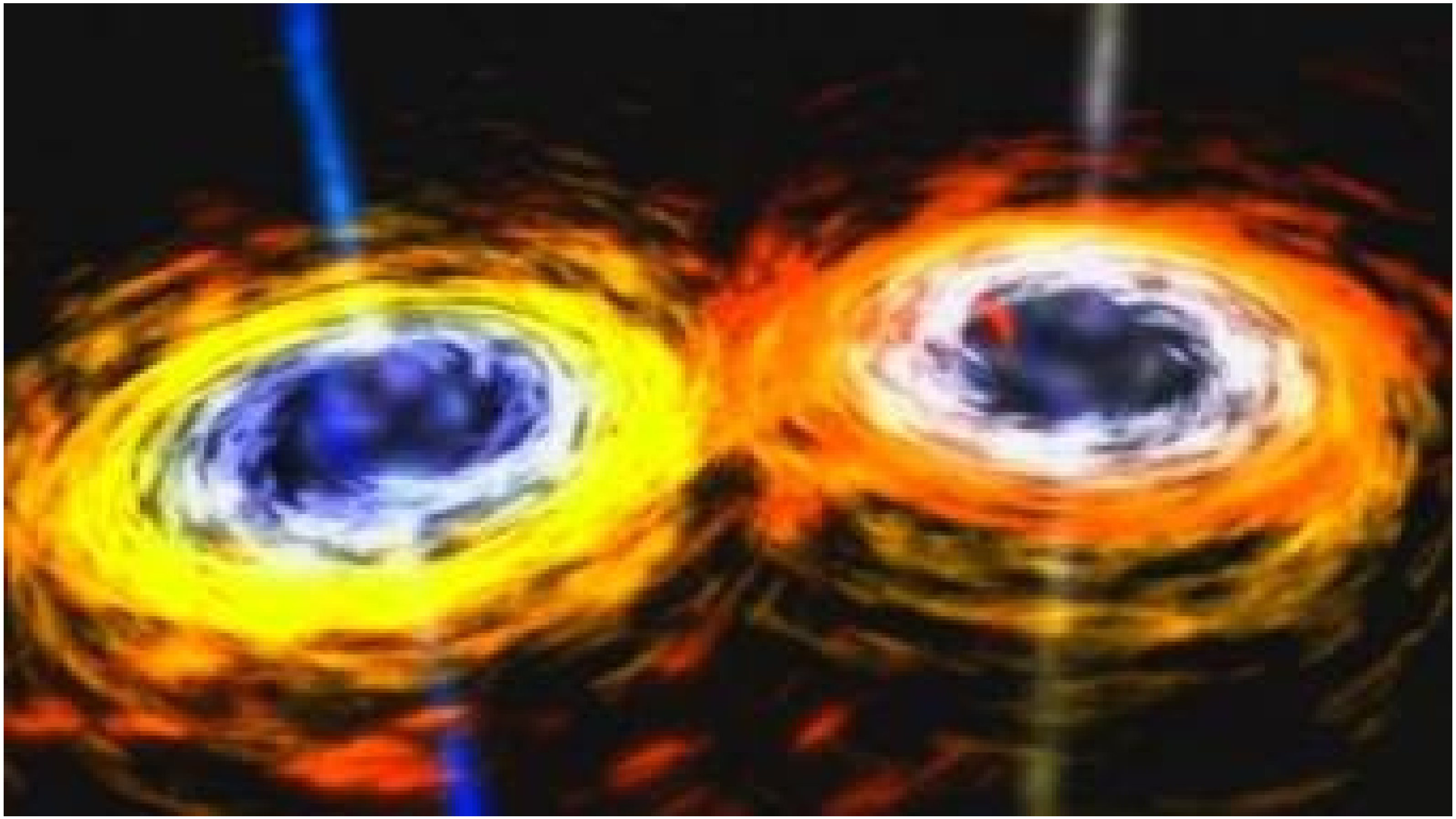
Boselli & AD-T, Physical Review C **92** (2015) 044610

- **Wave-packet dynamics** is a useful tool for modelling low-energy fusion dynamics of weakly bound nuclei.

- **Complete & incomplete fusion** can unambiguously be separated in the **configuration space**.

- **A three-dimensional quantum dynamical model** using wave-packet dynamics is being developed.

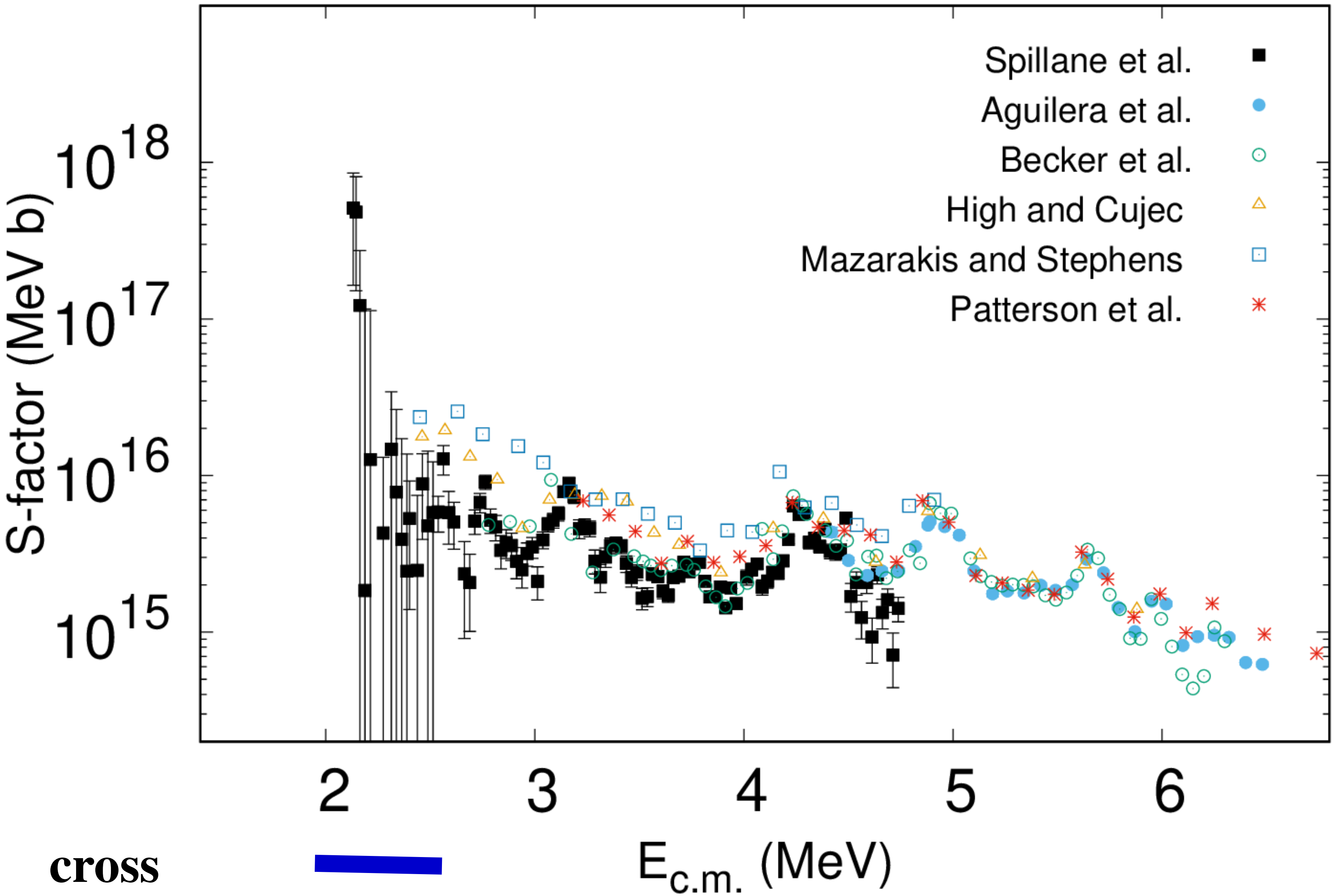
How do two ^{12}C nuclei fuse at sub-barrier energies?



Picture taken from BBC News

AD-T & Wiescher, Physical Review C **97** (2018) 055802

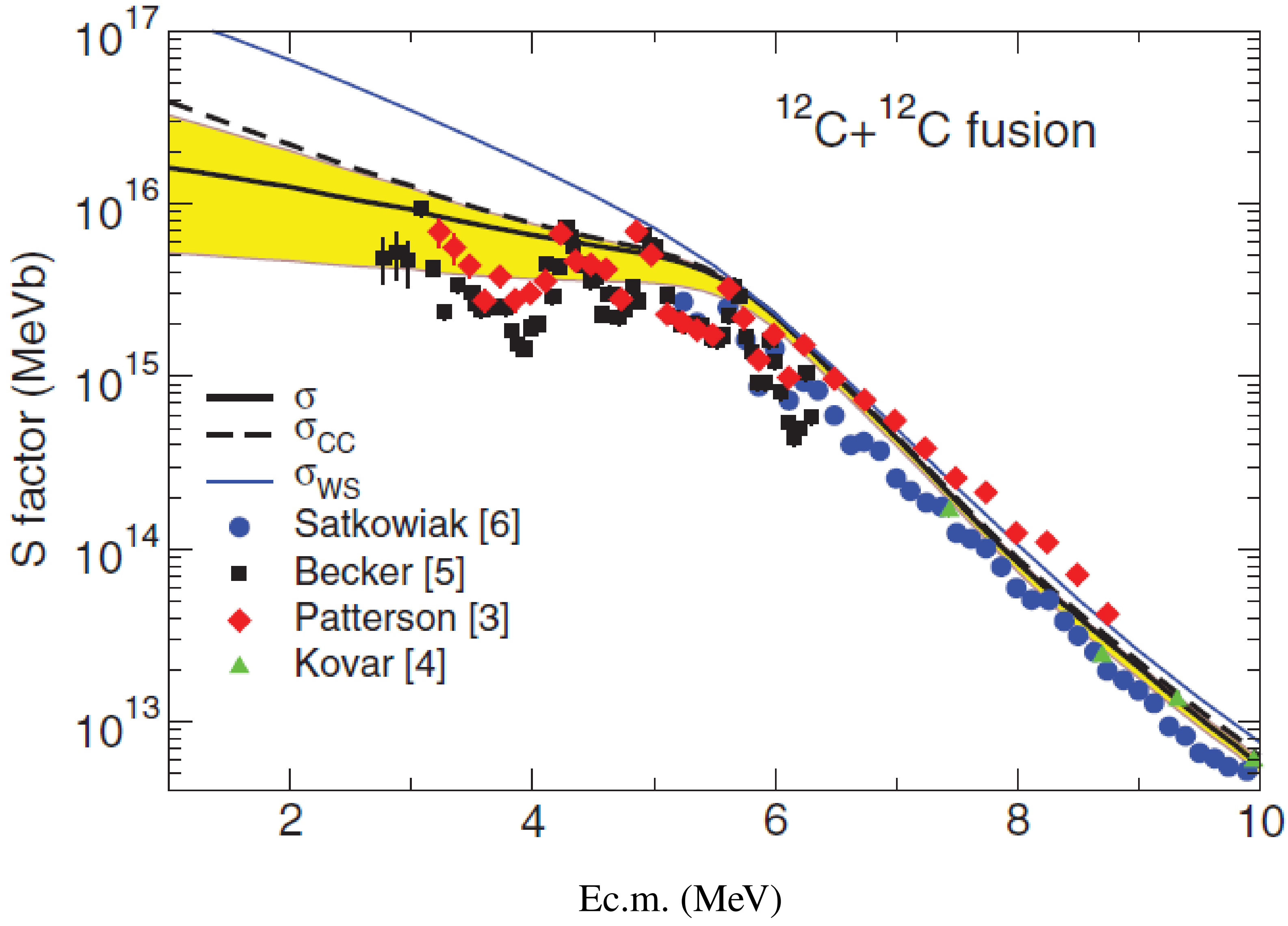
Astrophysical S-Factor for $^{12}C + ^{12}C$ Fusion



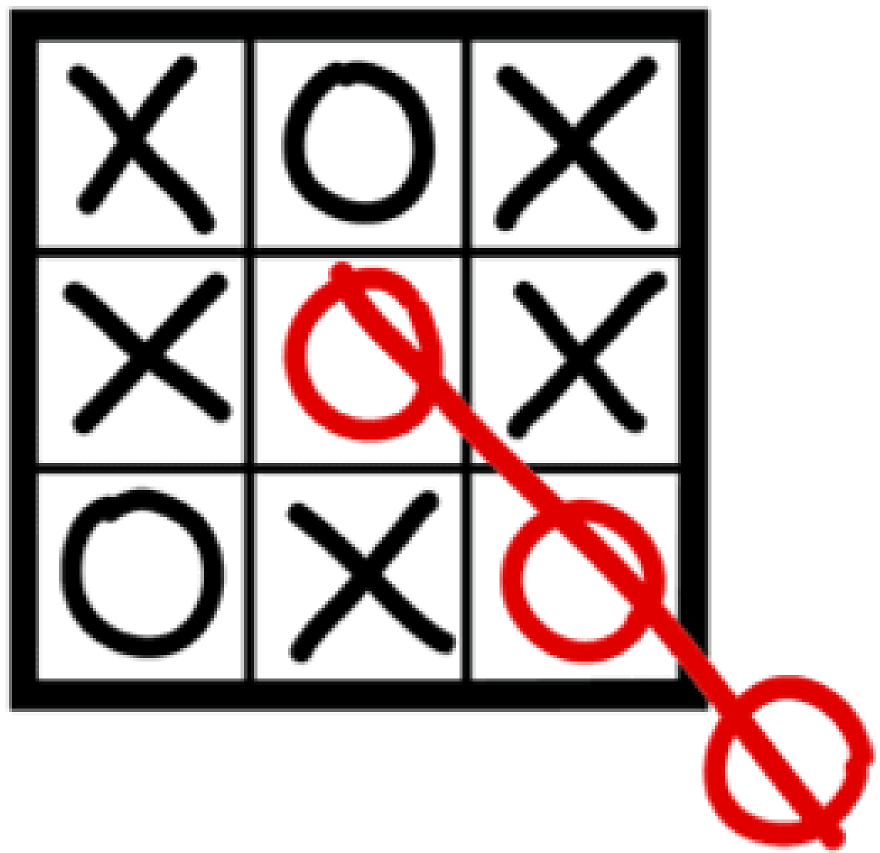
cross section 1pb 1nb

Coupled-Channels Calculations for $^{12}C + {}^{12}C$

Jiang, Esbensen et al., PRL **110** (2013) 072701

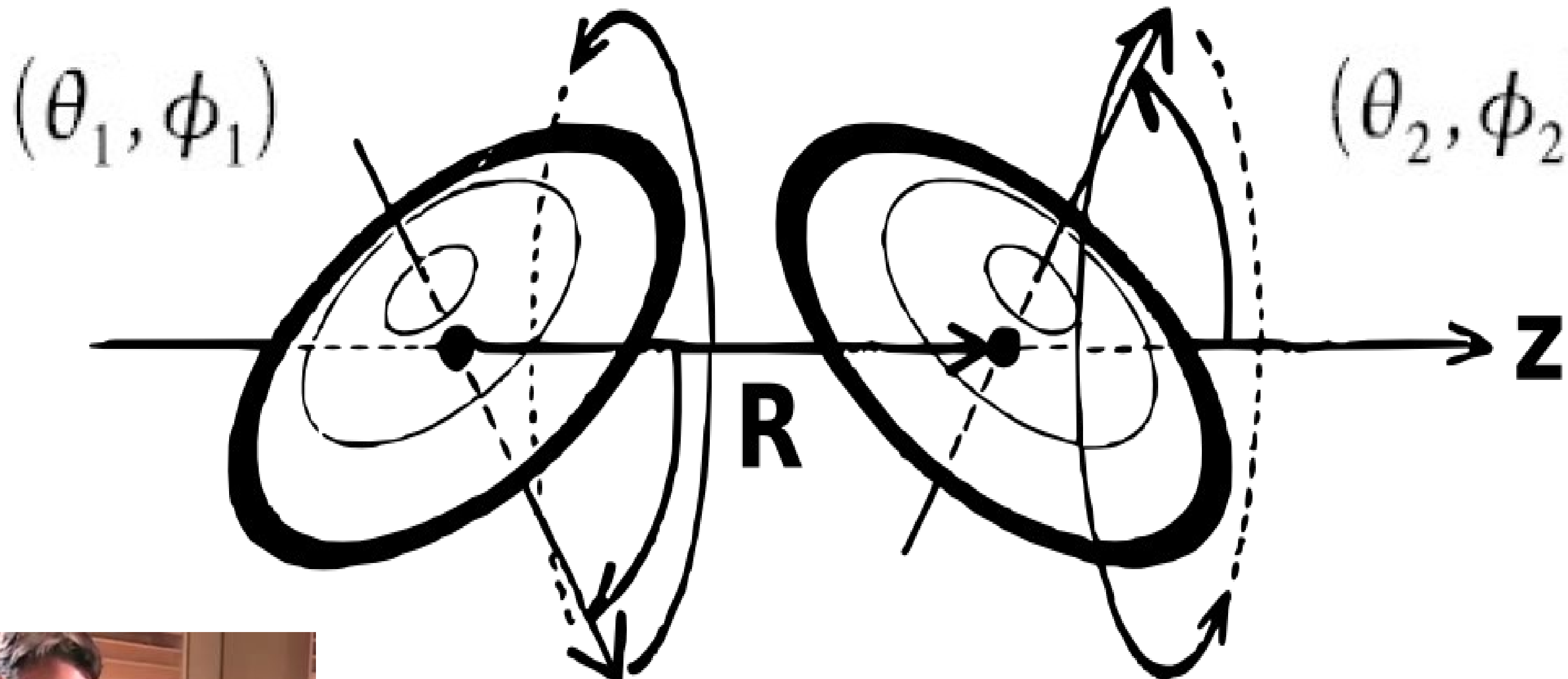


THINK OUTSIDE THE BOX



The $^{12}C + {}^{12}C$ Molecular Structure

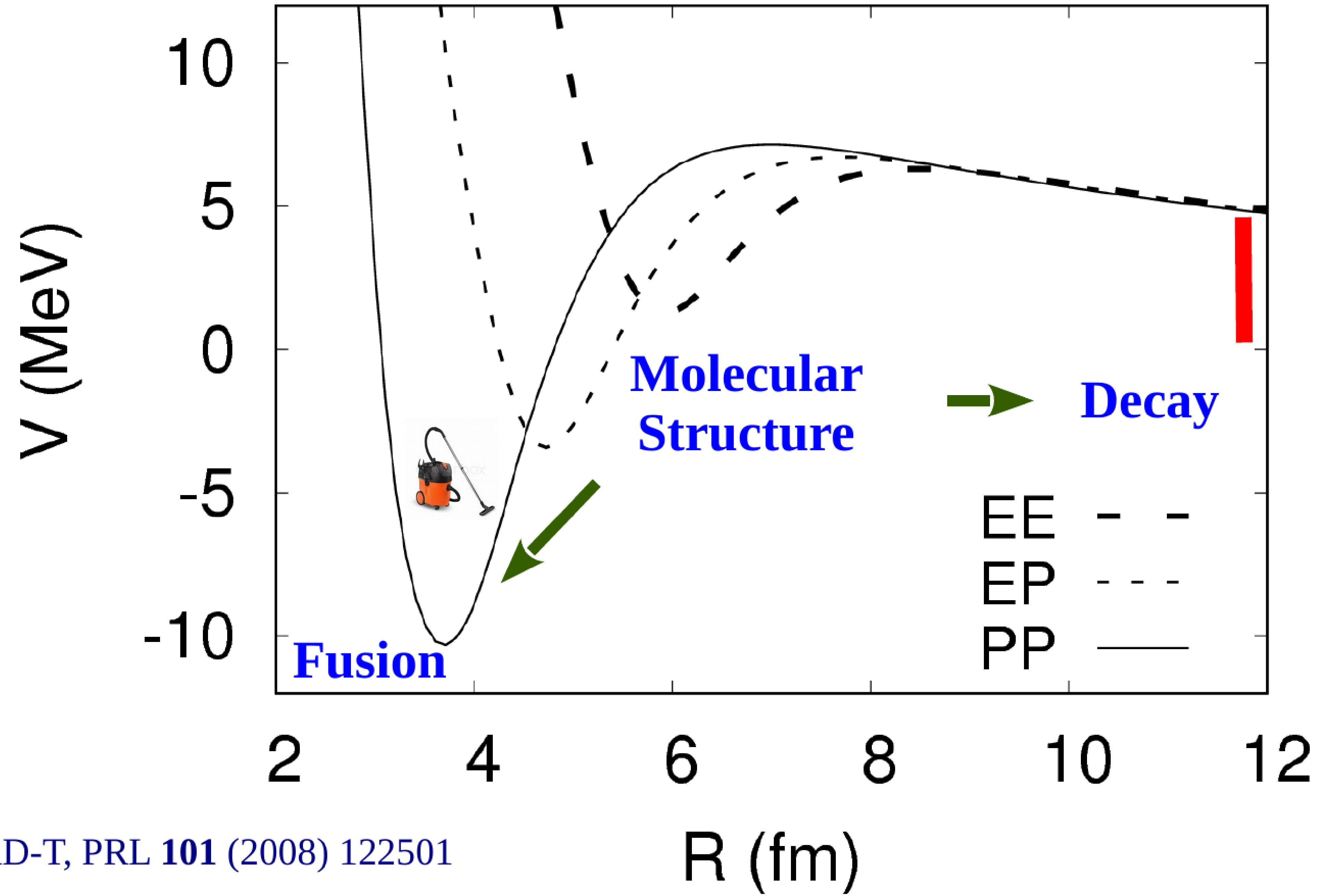
Greiner, Park & Scheid, in Nuclear Molecules, World Scientific, 1994



Quadrupole deformation of ^{12}C: ~ **- 0.5**

How does this molecular structure affect low-energy fusion?

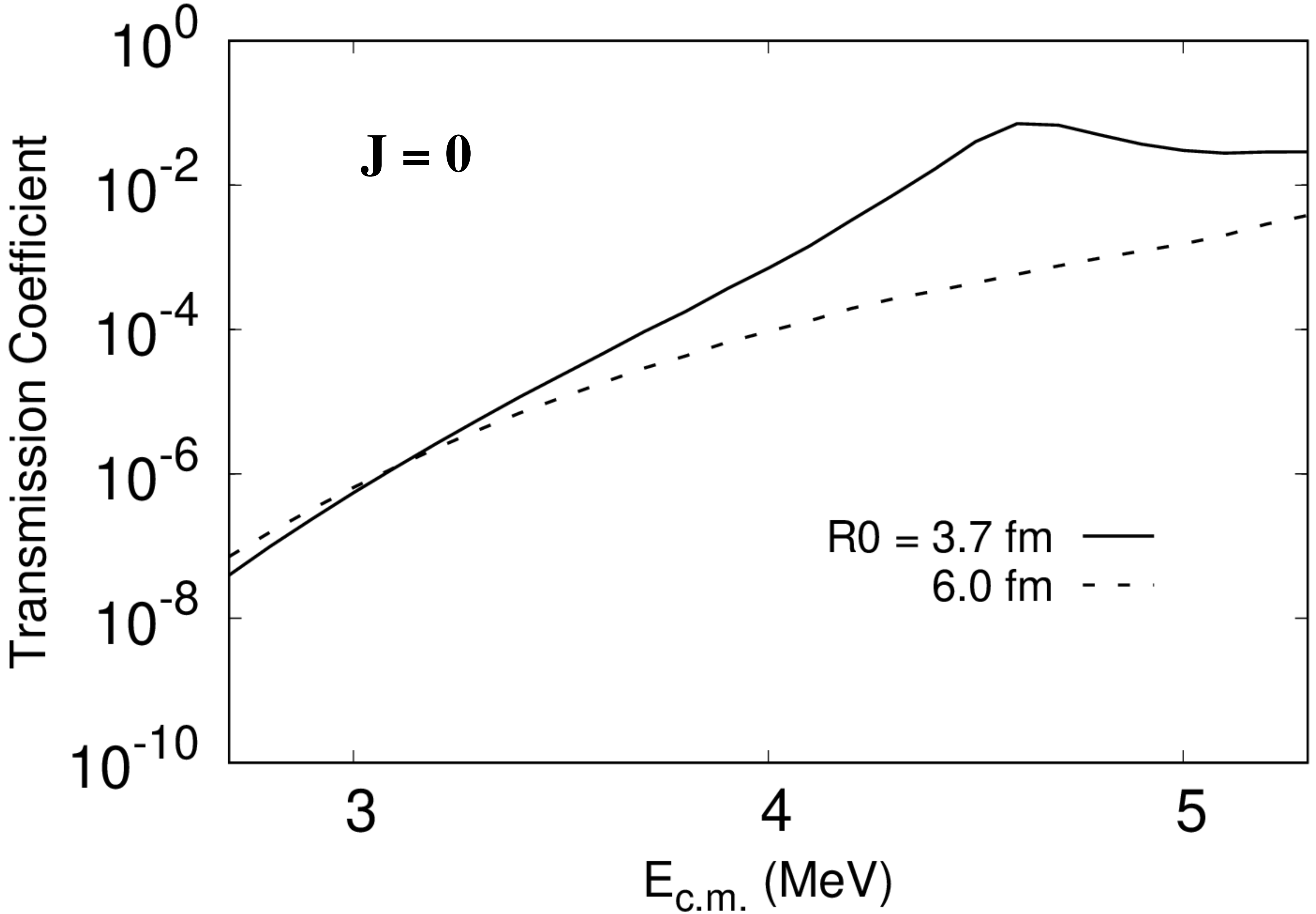
Collective Potential-Energy Landscape for $^{12}C + ^{12}C$



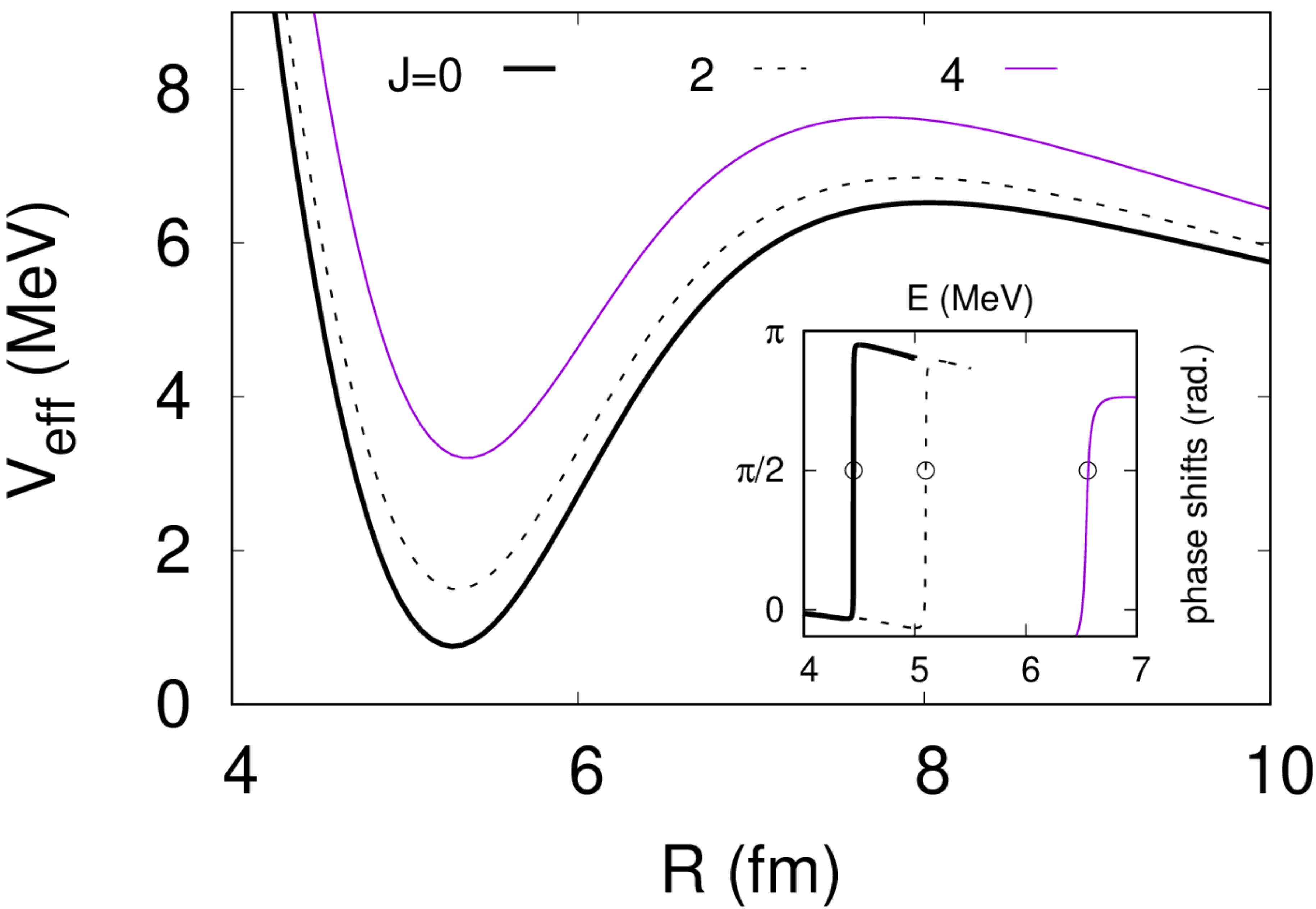
AD-T, PRL **101** (2008) 122501

Moeller & Iwamoto, NPA **575** (1994) 381

Role of the imaginary fusion potential in the transmission coefficient



Phase shift analysis of effective potentials for $^{12}C + ^{12}C$



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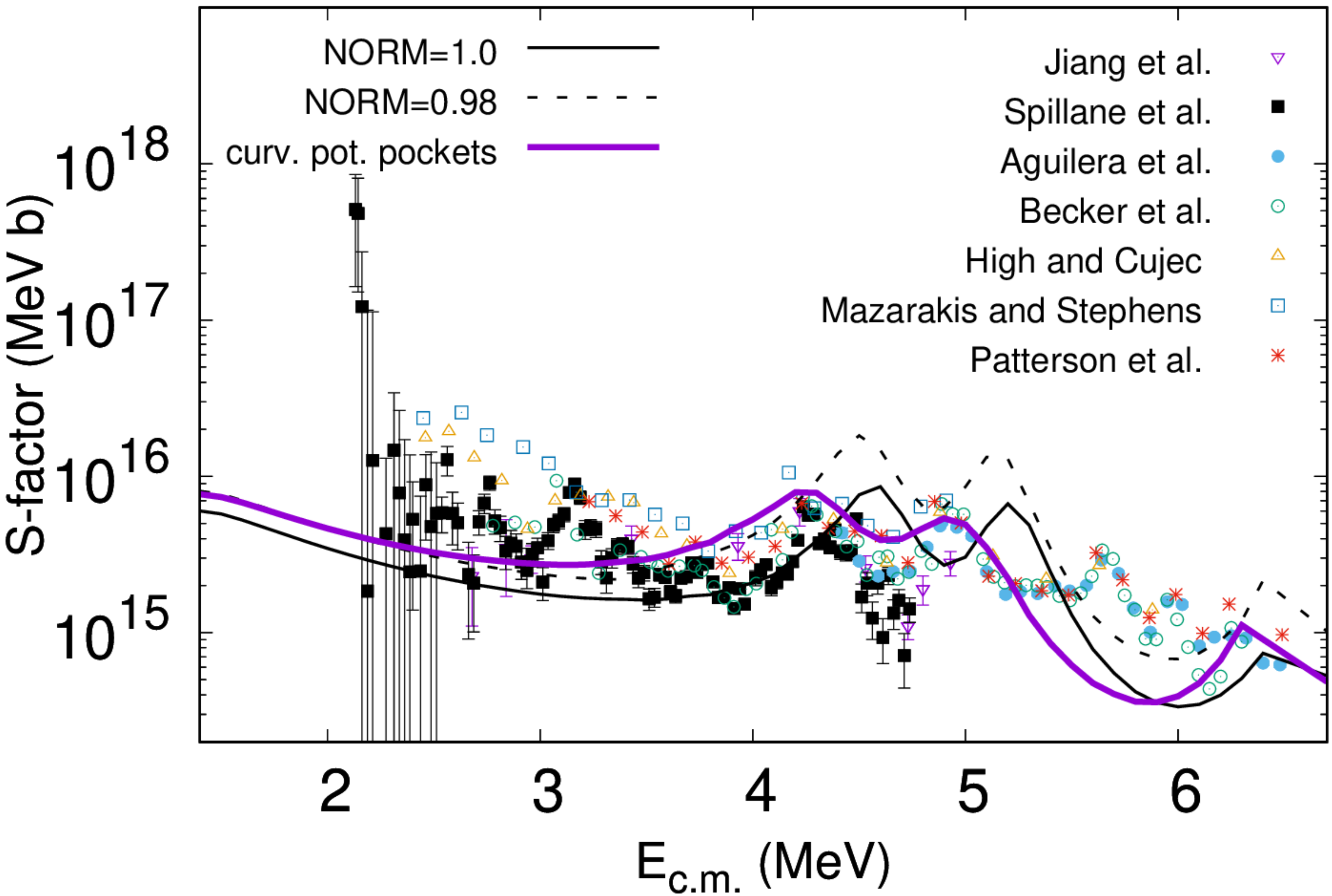


Summarising

AD-T & Wiescher, Physical Review C **97** (2018) 055802

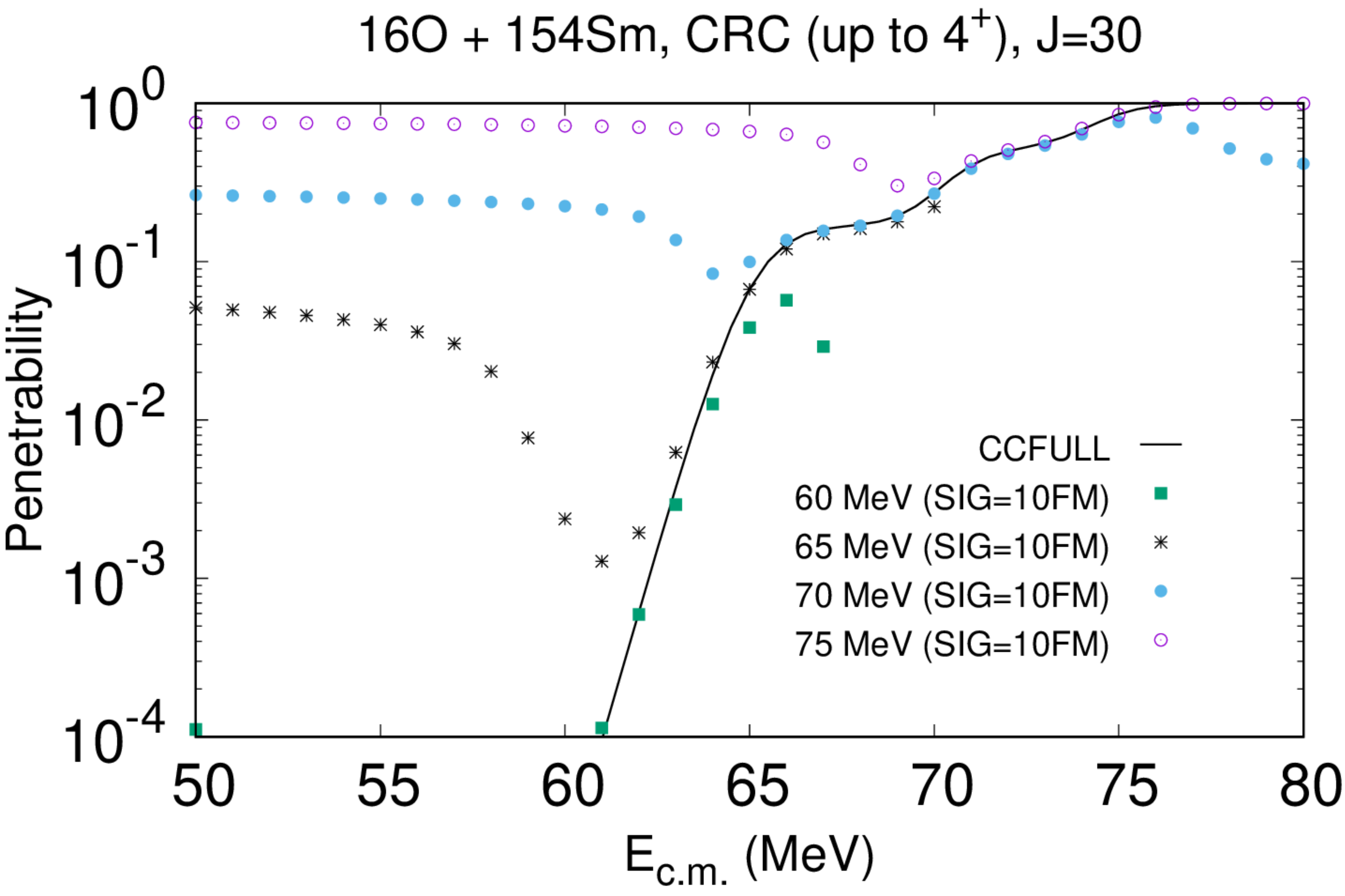
- The **fusion imaginary potential** for *specific* dinuclear configurations is crucial for the appearance of resonances.

- **Three resonant structures** are revealed in the calculations, reproducing similar structures in the experimental data.

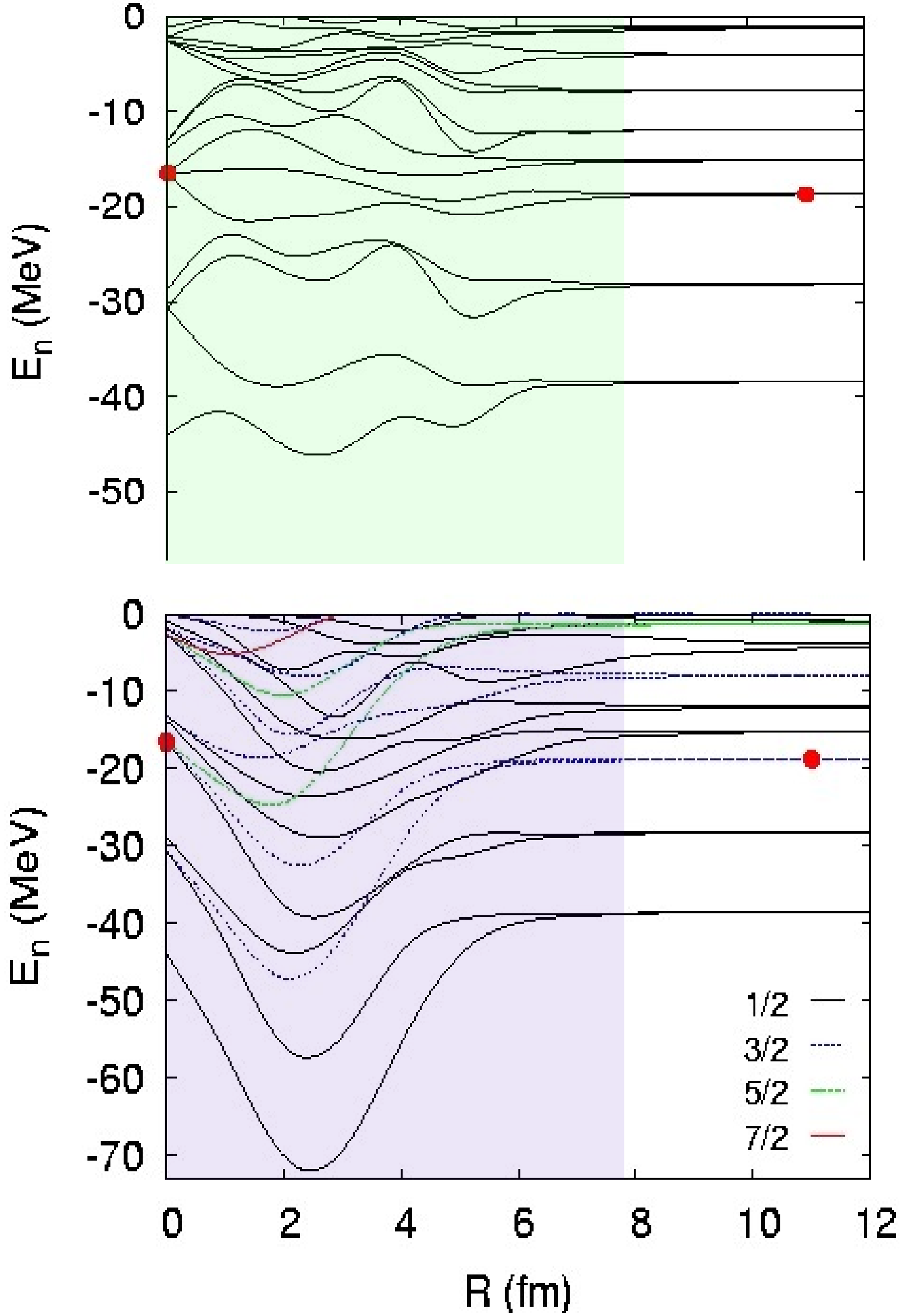
- **Resonant structures** in the experimental data that are not explained may be due to **cluster effects** in the nuclear molecule.

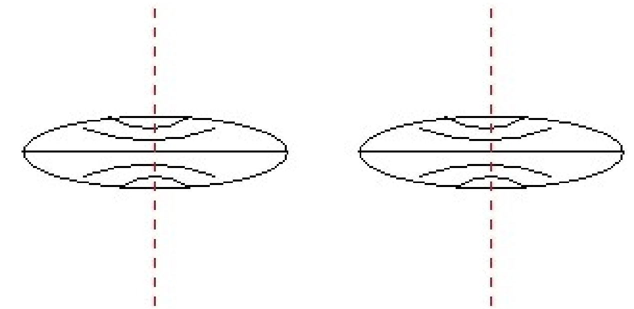
EXTRA SLIDES

Wave-packet dynamics & stationary CRC



Sensitivity of Molecular Shell Structure to the ^{12}C Alignment

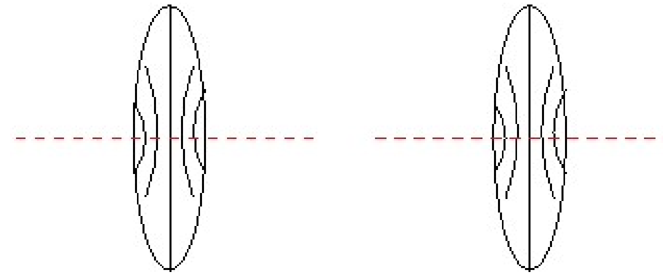




$$V = \sum_{s=1}^{2} e^{-i\mathbf{R}_s \hat{k}}\, \hat{U}(\Omega_s)\, V_s\, \hat{U}^{-1}(\Omega_s)\, e^{i\mathbf{R}_s \hat{k}}$$

$$V_s \approx \sum_{\nu\mu}^{N} |s\nu\rangle\, V^s_{\nu\mu}\, \langle s\mu|$$

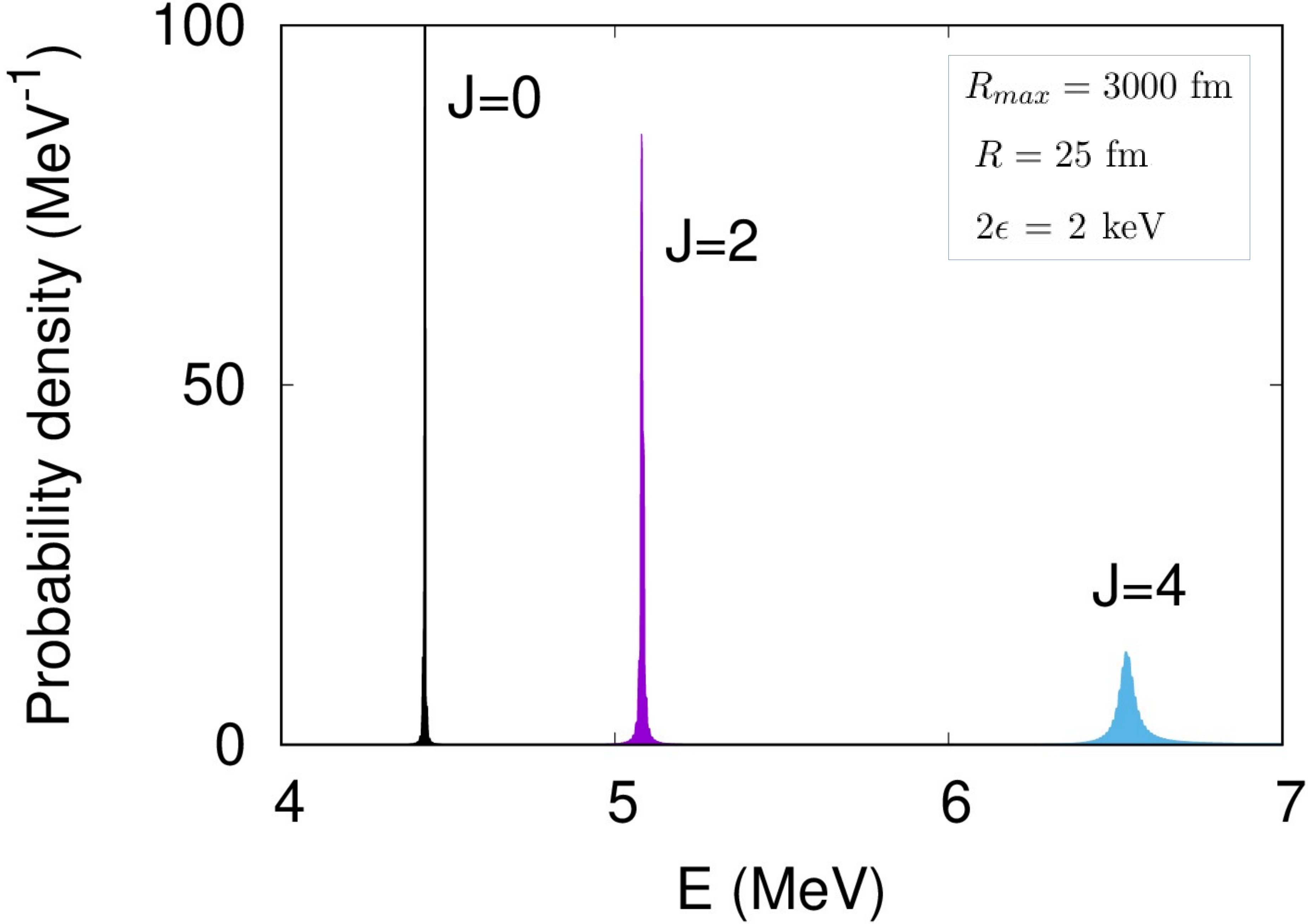
Potential Separable Expansion Method



AD-T, PRL **101** (2008) 122501

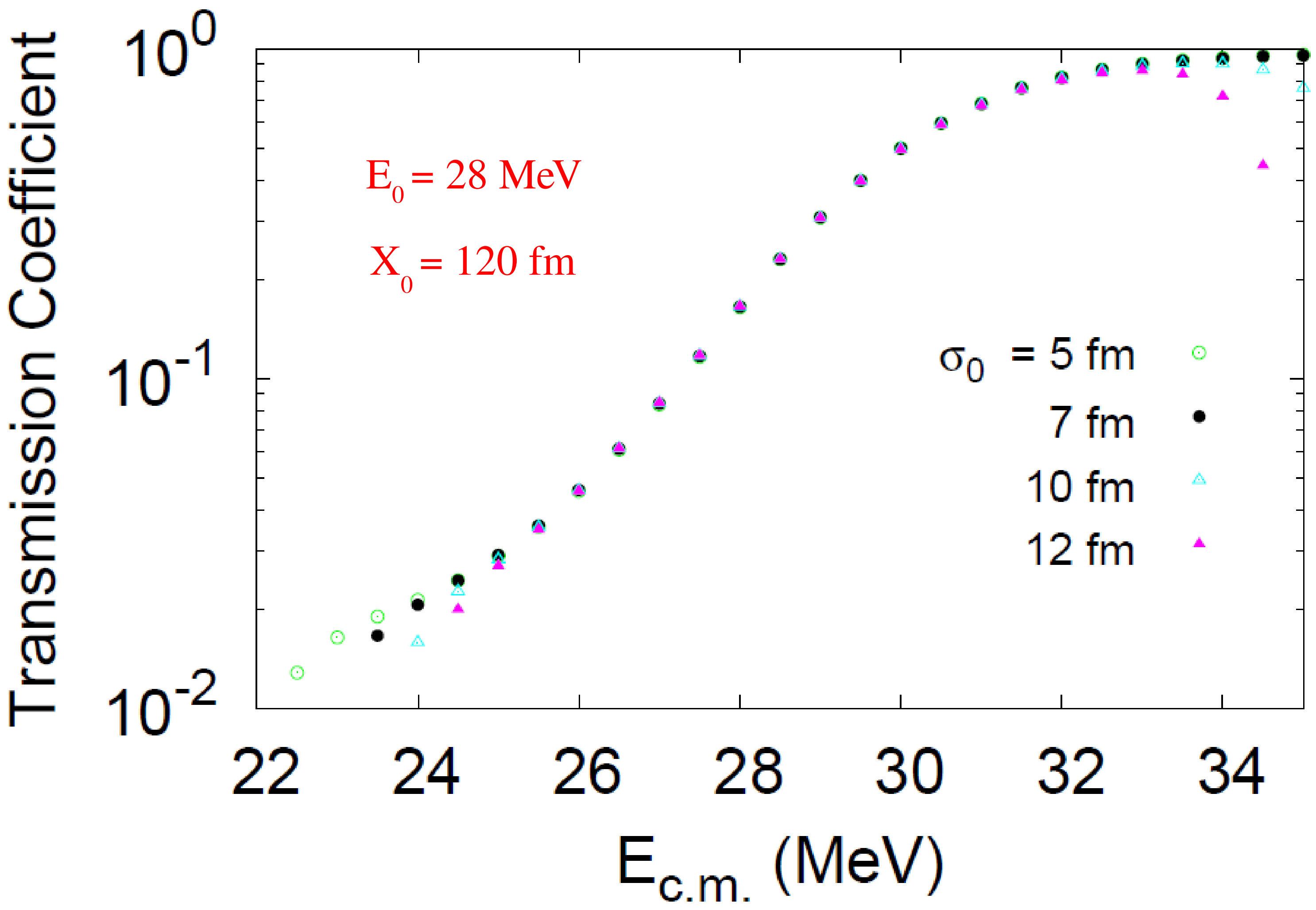
Probability Density Function

AD-T & Tostevin, arXiv: 1809.10517v1



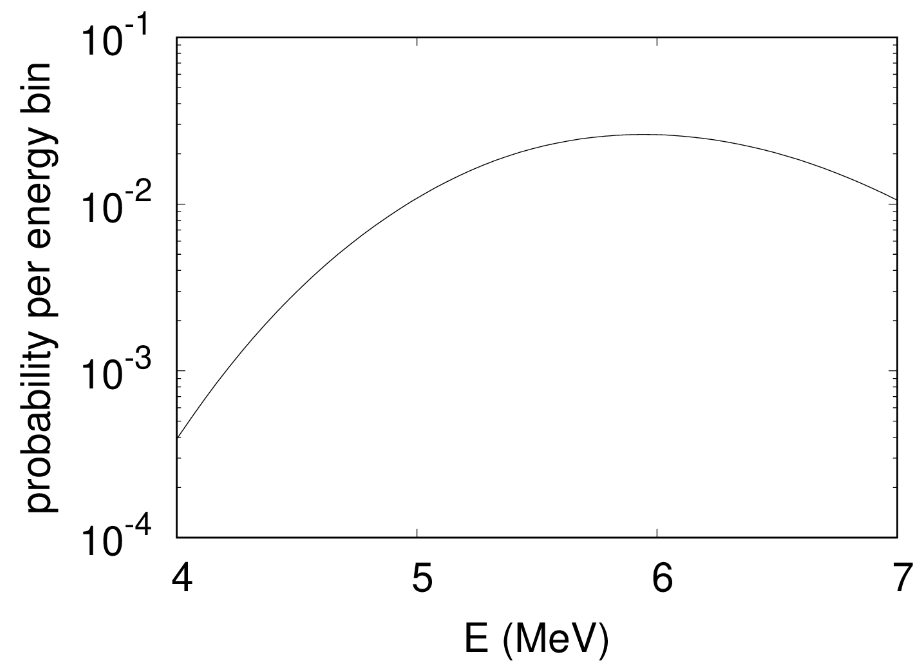
Results

♦ Energy-resolved **total transmission** for different values of the **spatial width** of the **initial wave packet**



Energy Projection of the Wave Function

Schafer & Kulander,
PRA **42** (1990) 5794



- **Energy spectra** of $\Psi(t)$ as expectation values of **the window operator**

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- $\mathcal{P}(E_k) = \langle\Psi|\hat{\Delta}|\Psi\rangle$, for instance, **n = 2** :

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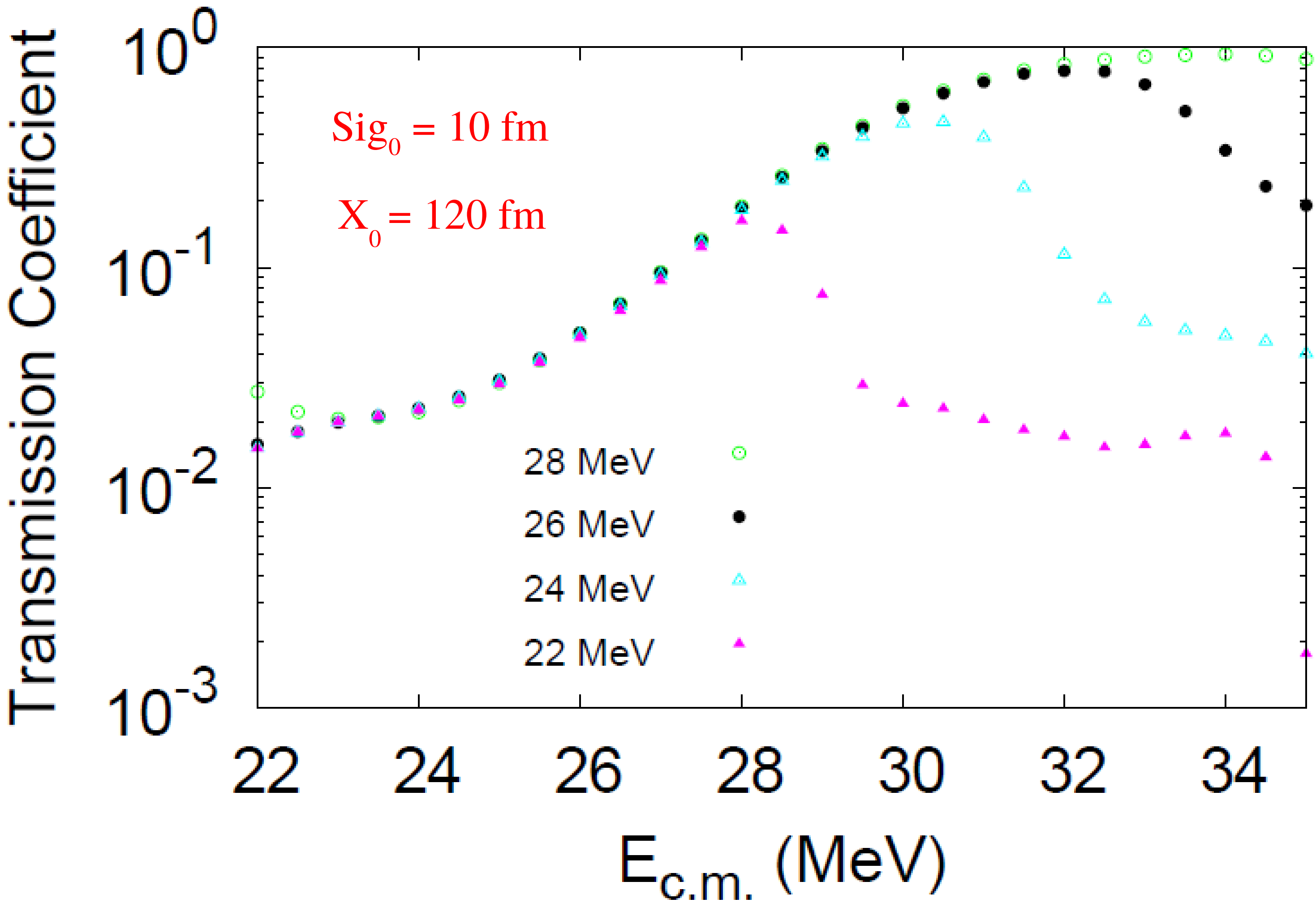
$$\rightarrow \quad \boxed{\mathcal{P}(E_k) = \langle\chi_k|\chi_k\rangle}$$

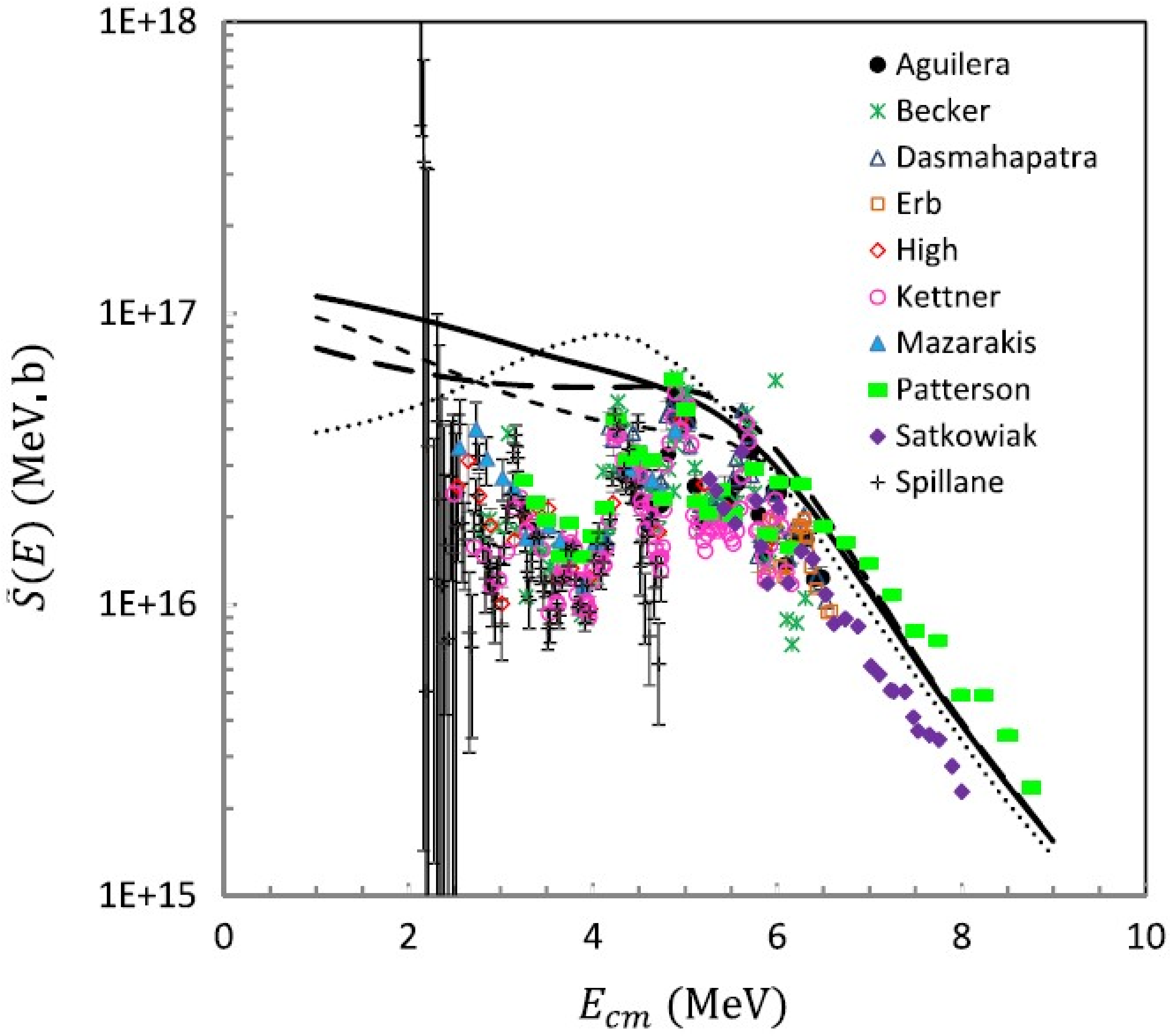
Results

♦ Energy-resolved **total transmission** for different values of the **mean energy** of the **initial wave packet**



Coupled-Channels Calculations for ^{12}C + ^{12}C

Assuncao & Descouvemont, PLB **723** (2013) 355



Fusion Cross Section & Astrophysical S-Factor

$$S(E) = \sigma(E)\,\boxed{E\ \exp\,(\,2\,\pi\,\eta\,)}$$

Structural factor [MeV barn]

Fusion cross section [barn = 10^{-28} m^2]

$$\eta = (\frac{\mu}{2})^{1/2}\,\frac{Z_1\,Z_2\,e^2}{\hbar\,E^{1/2}}$$

Sommerfeld parameter

S(E) represents the fusion cross section free of Coulomb suppression, which is adequate for extrapolation towards stellar energies

Kinetic-Energy of Two Deformed Colliding Nuclei

Gatti *et al.*, JCP **123** (2005) 174311

$$
\begin{aligned}
\frac{2\hat{T}}{\hbar^2} \;=\;& -\frac{1}{\mu}\frac{\partial^2}{\partial R^2} + \left(\frac{1}{I_1} + \frac{1}{\mu R^2}\right)\hat{j}_1^2 + \left(\frac{1}{I_2} + \frac{1}{\mu R^2}\right)\hat{j}_2^2 \\
& + \frac{1}{\mu R^2}\big[\hat{j}_{1,+}\hat{j}_{2,-} + \hat{j}_{1,-}\hat{j}_{2,+} + J(J+1) \\
& - 2k_1^2 - 2k_1 k_2 - 2k_2^2\big] - \boxed{\frac{C_+(J,K)}{\mu R^2}(\hat{j}_{1,+} + \hat{j}_{2,+})} \\
& - \boxed{\frac{C_-(J,K)}{\mu R^2}(\hat{j}_{1,-} + \hat{j}_{2,-})}
\end{aligned}
$$

Coriolis interaction

μ is the reduced mass for the radial motion,
I_i is the ^{12}C rotational inertia,
J is the total angular momentum with projection $K = k_1 + k_2$,
$C_\pm(J,K) = \sqrt{J(J+1) - K(K\pm 1)}$,
$\hat{j}_i^2 = -\frac{1}{\sin\theta_i}\frac{\partial}{\partial\theta_i}\sin\theta_i\frac{\partial}{\partial\theta_i} + \frac{k_i^2}{\sin^2\theta_i}$,
$\hat{j}_{i,\pm} = \pm\frac{\partial}{\partial\theta_i} - k_i\cot\theta_i$, with $k_i \rightarrow k_i \pm 1$.

Initial state $\Psi(t=0)$: the ^{12}C nuclei are well separated

$$\Psi_0(R,\theta_1,k_1,\theta_2,k_2) = \chi_0(R)\,\psi_0(\theta_1,k_1,\theta_2,k_2),$$

Radial motion

Internal rotational motion

$$\chi_0(R) = (\sqrt{\pi}\sigma)^{-1/2}\,\exp\left[-\frac{(R-R_0)^2}{2\sigma^2}\right] e^{iP_0(R-R_0)},$$

$$\begin{aligned}\psi_0(\theta_1,k_1,\theta_2,k_2) \;=\;& \big[\zeta_{j_1,m_1}(\theta_1,k_1)\zeta_{j_2,m_2}(\theta_2,k_2) \\ &+(-1)^J\zeta_{j_2,-m_2}(\theta_1,k_1)\zeta_{j_1,-m_1}(\theta_2,k_2)\big] \\ &/\sqrt{2+2\,\delta_{j_1,j_2}\delta_{m_1,-m_2}},\end{aligned}$$

where $\zeta_{j,m}(\theta,k) = \sqrt{\frac{(2j+1)(j-m)!}{2\,(j+m)!}}\,P_j^m(\cos\theta)\,\delta_{km}$,
and P_j^m are associated Legendre functions.

Time Propagation of the Wave Function

$$|\Psi_J(t)\rangle = \underbrace{e^{-i\,\hat{H}\,t/\hbar}}_{\text{evolution operator}}\,|\Psi_J(0)\rangle$$

The evolution operator is represented as a convergent series of modified Chebyshev polynomials

Tannor, Quantum Mechanics from a Time-Dependent Perspective, USB, 2007

Power Spectrum of the Wave Function

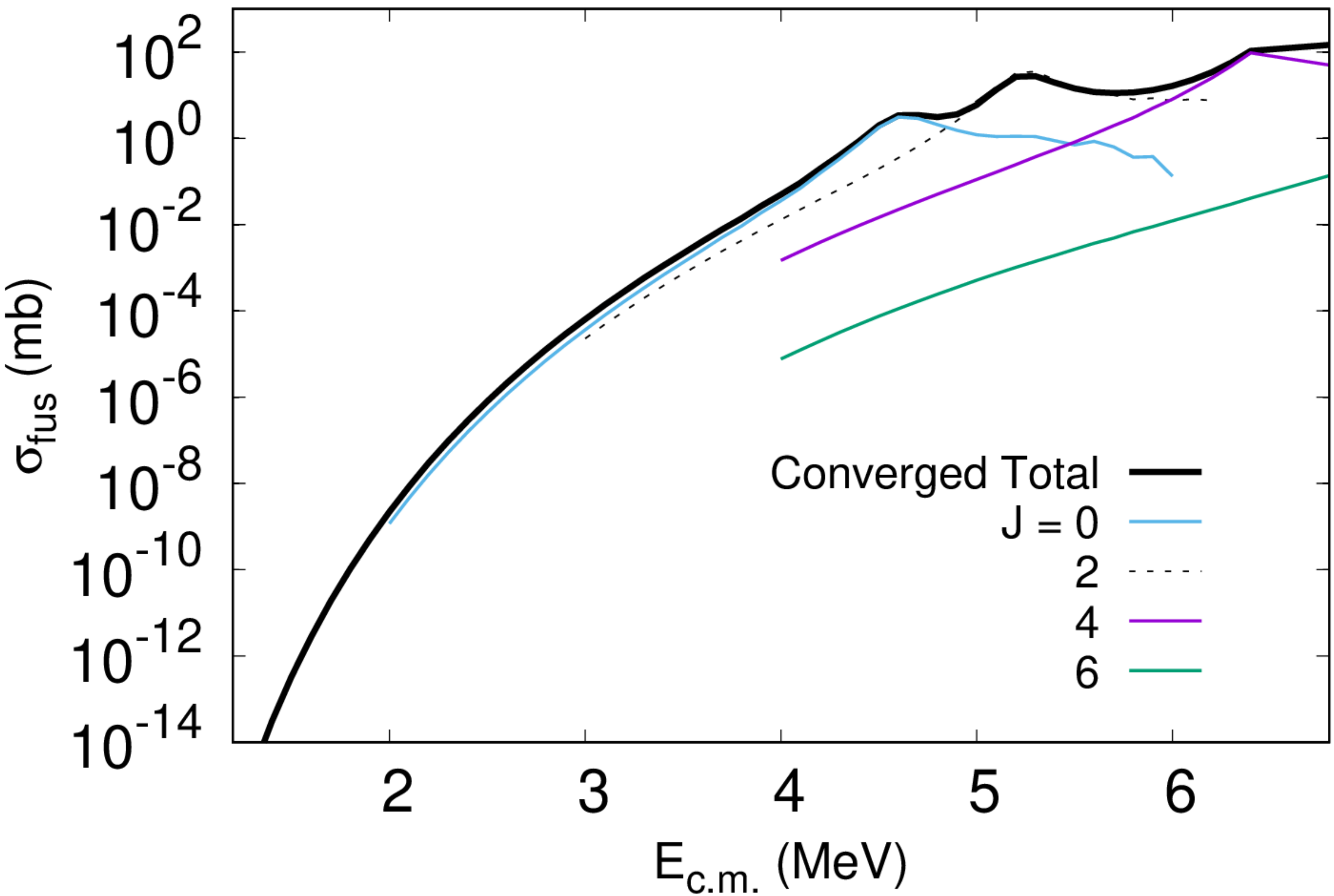
$$\mathcal{P}(E) = \langle \Psi(t) | \underbrace{\delta(E - \hat{H})}_{\text{Energy projector}} | \Psi(t) \rangle$$

Reflection & Transmission Coefficients

$$\mathcal{R}(E) = \frac{\mathcal{P}^{final}(E)}{\mathcal{P}^{initial}(E)}$$

$$T(E) = 1 - \mathcal{R}(E)$$

Fusion Excitation Function for $^{12}C + ^{12}C$



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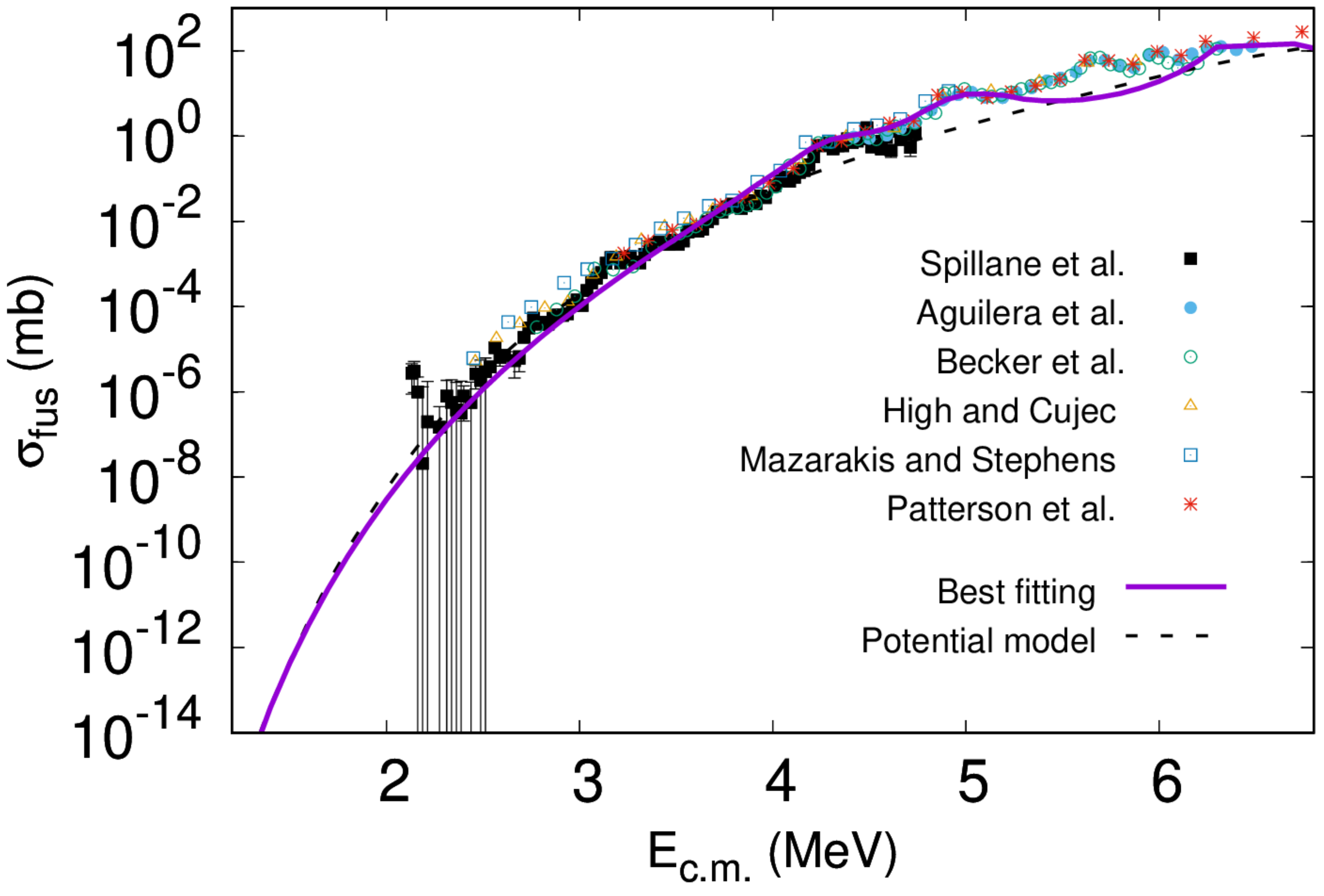
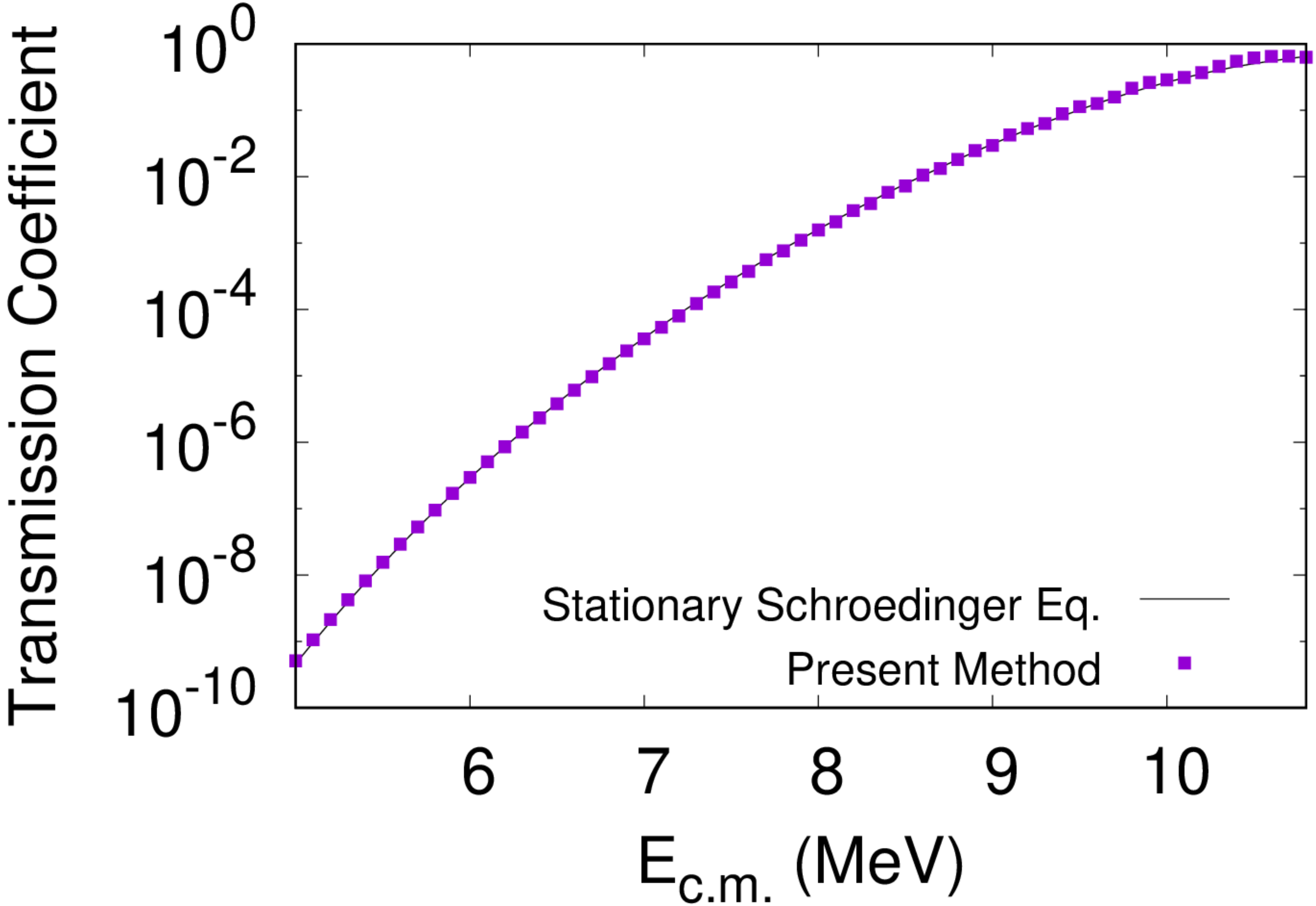


Transmission coefficients for $^{16}O + {}^{16}O$ central collisions

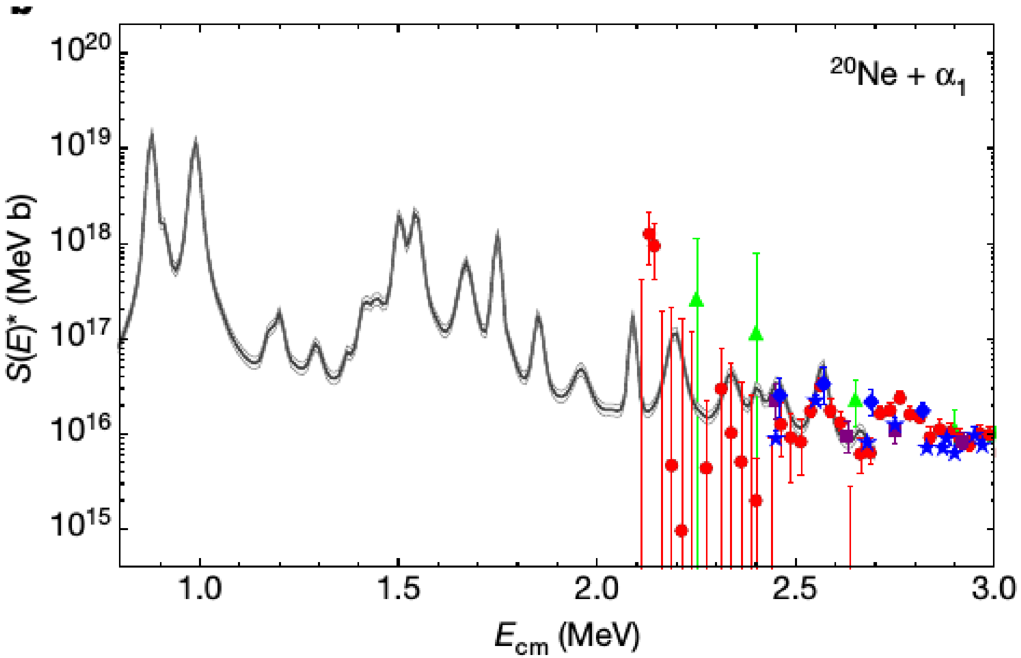


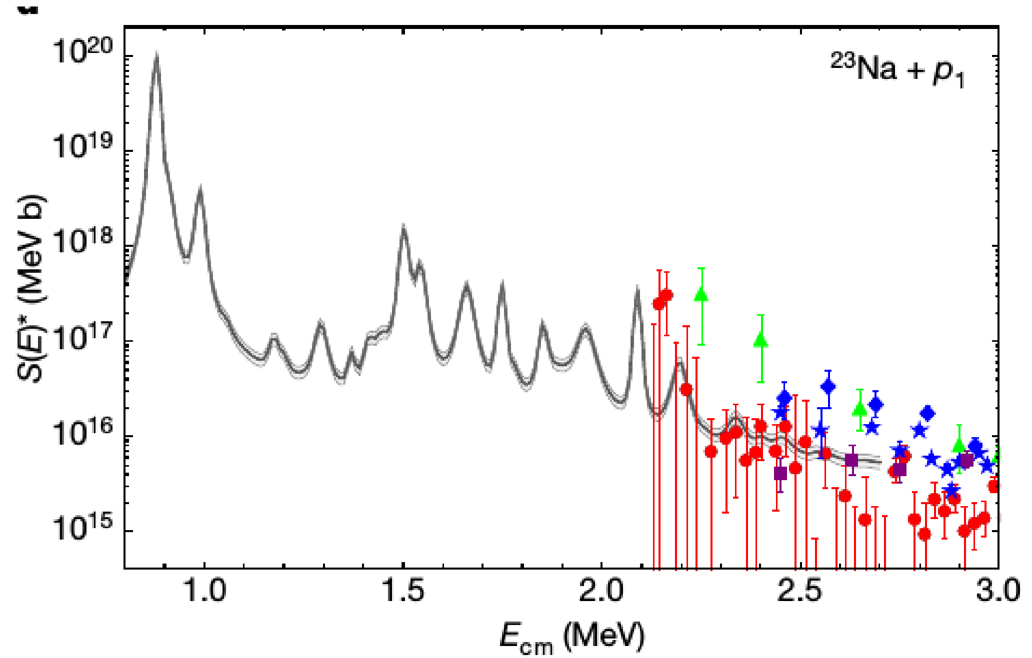
LETTER

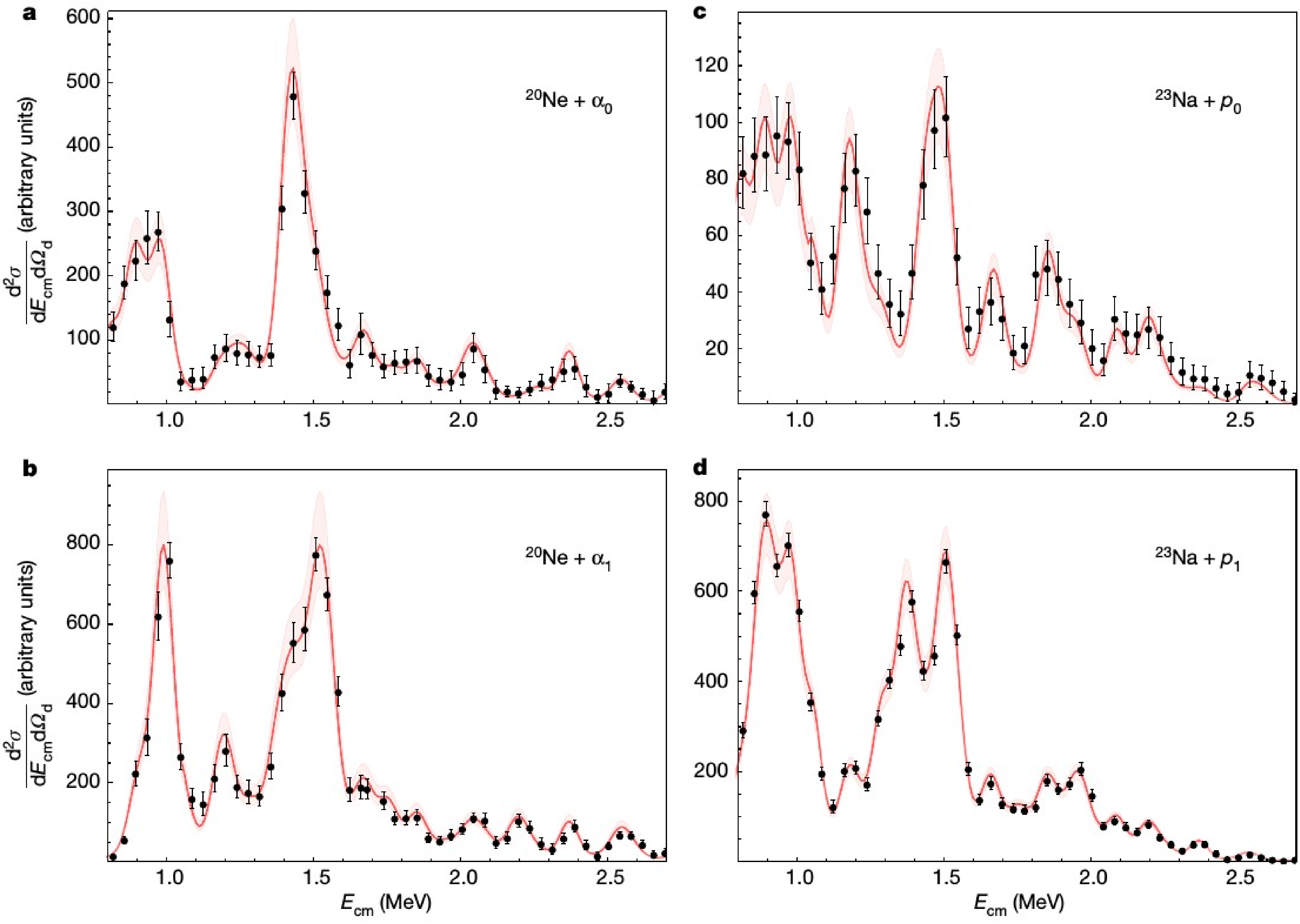
https://doi.org/10.1038/s41586-018-0149-4

An increase in the $^{12}C + ^{12}C$ fusion rate from resonances at astrophysical energies

A. Tumino[1,2]*, C. Spitaleri[2,3], M. La Cognata[2], S. Cherubini[2,3], G. L. Guardo[2,4], M. Gulino[1,2], S. Hayakawa[2,5], I. Indelicato[2], L. Lamia[2,3], H. Petrascu[4], R. G. Pizzone[2], S. M. R. Puglia[2], G. G. Rapisarda[2], S. Romano[2,3], M. L. Sergi[2], R. Spartá[2] & L. Trache[4]







a
b
c
d
$^{20}Ne + \alpha_0$
$^{20}Ne + \alpha_1$
$^{23}Na + p_0$
$^{23}Na + p_1$
$\frac{d^2\sigma}{dE_{cm}d\Omega_d}$ (arbitrary units)
E_{cm} (MeV)