Relating molecular structure & low-energy fusion through time-dependent wave-packet dynamics: the $^{12}C+^{12}C$ collision

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What I will tell you

- The **S-factor** & the **fusion cross section**
- The **^{12}C + ^{12}C molecule** & **sub-Coulomb fusion**
- Conclusions & Outlook

Fusion Cross Section & Astrophysical S-Factor

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

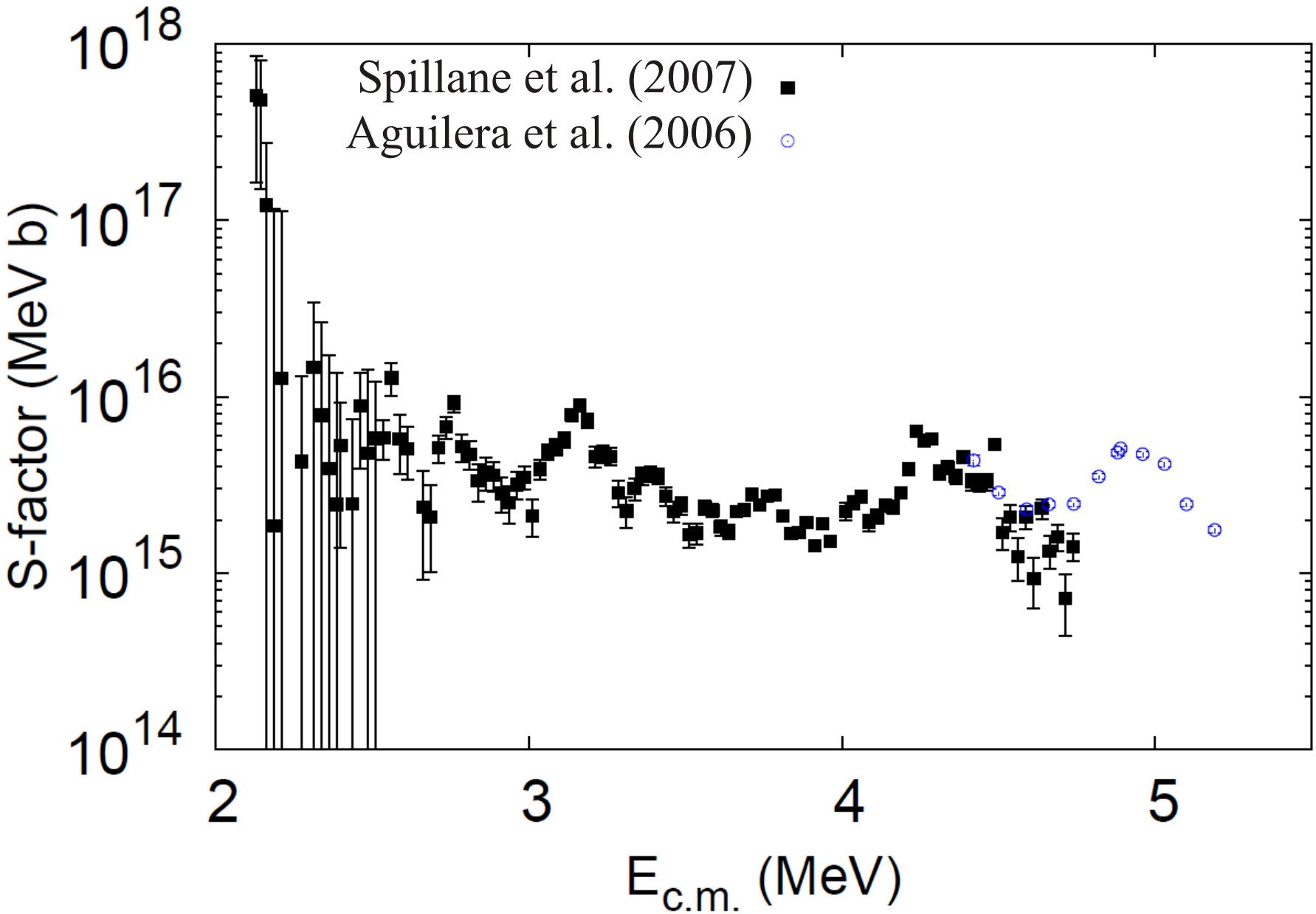
Structural factor — [MeV barn]

Fusion cross section — [barn]

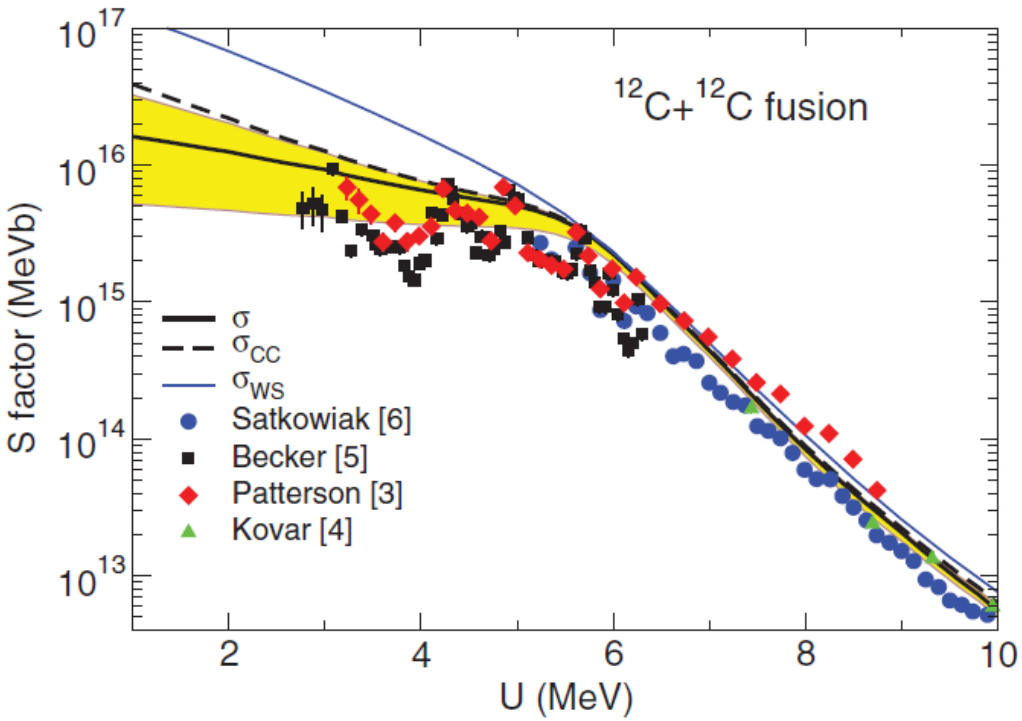
Sommerfeld parameter

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

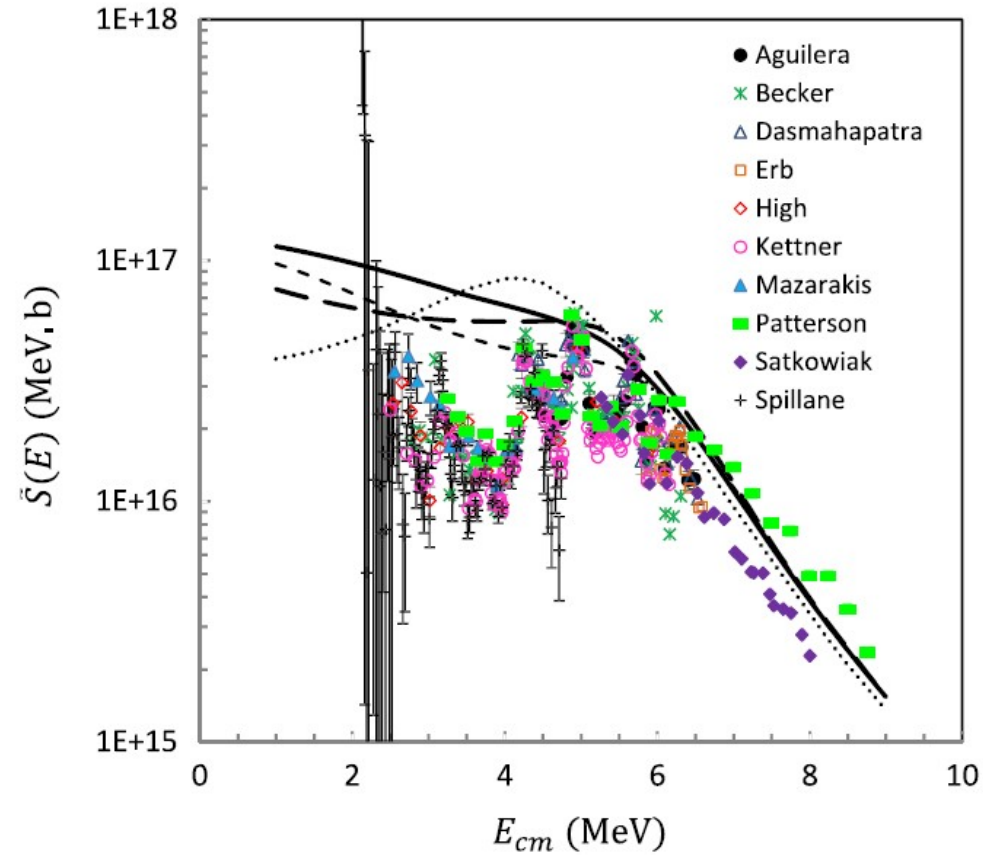
S-Factor Excitation Function for $^{12}C + ^{12}C$



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



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



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

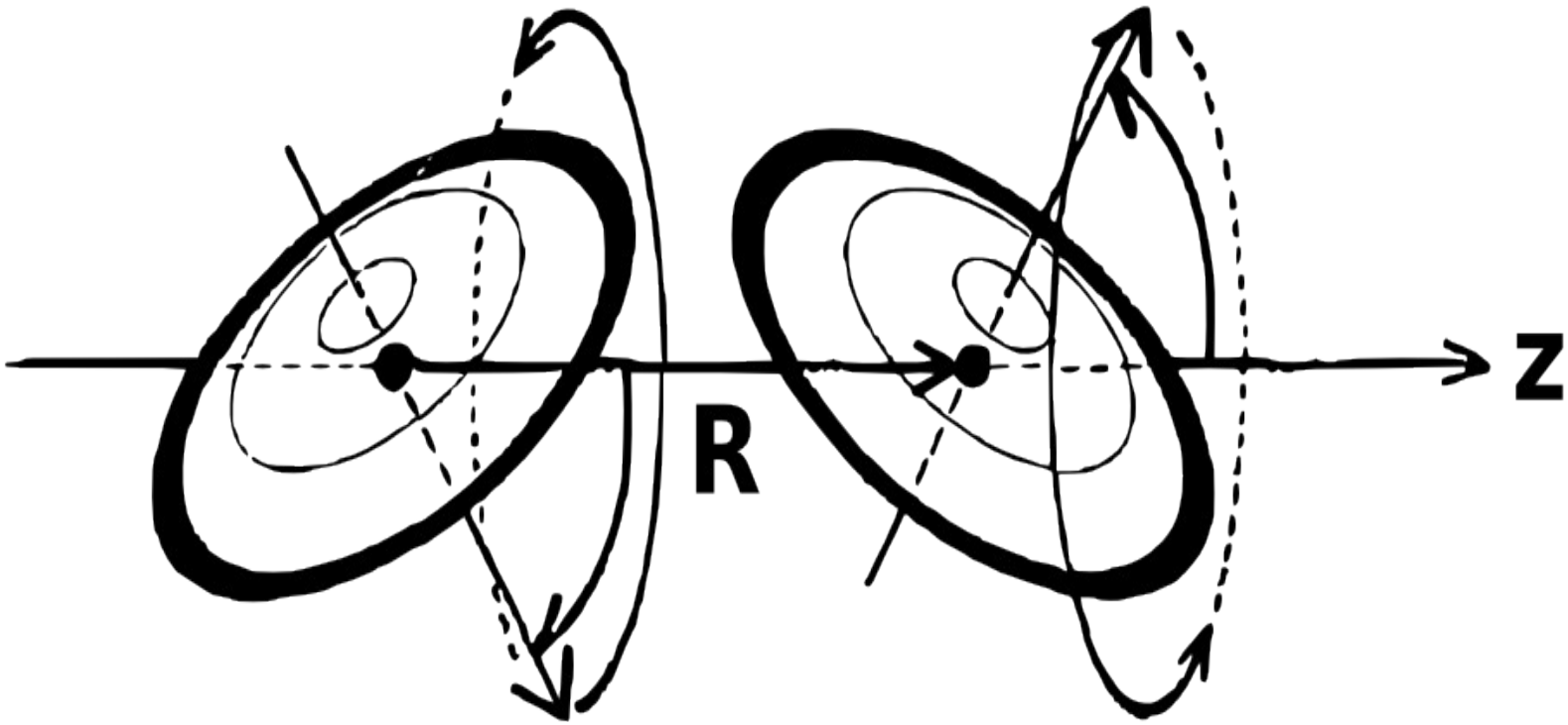
The physics of intermediate structure seems not to be included.

Excitations in the $^{12}C + ^{12}C$ Nuclear Molecule

P.O. Hess & P. Pereyra, Phys. Rev. C **42** (1990) 1632

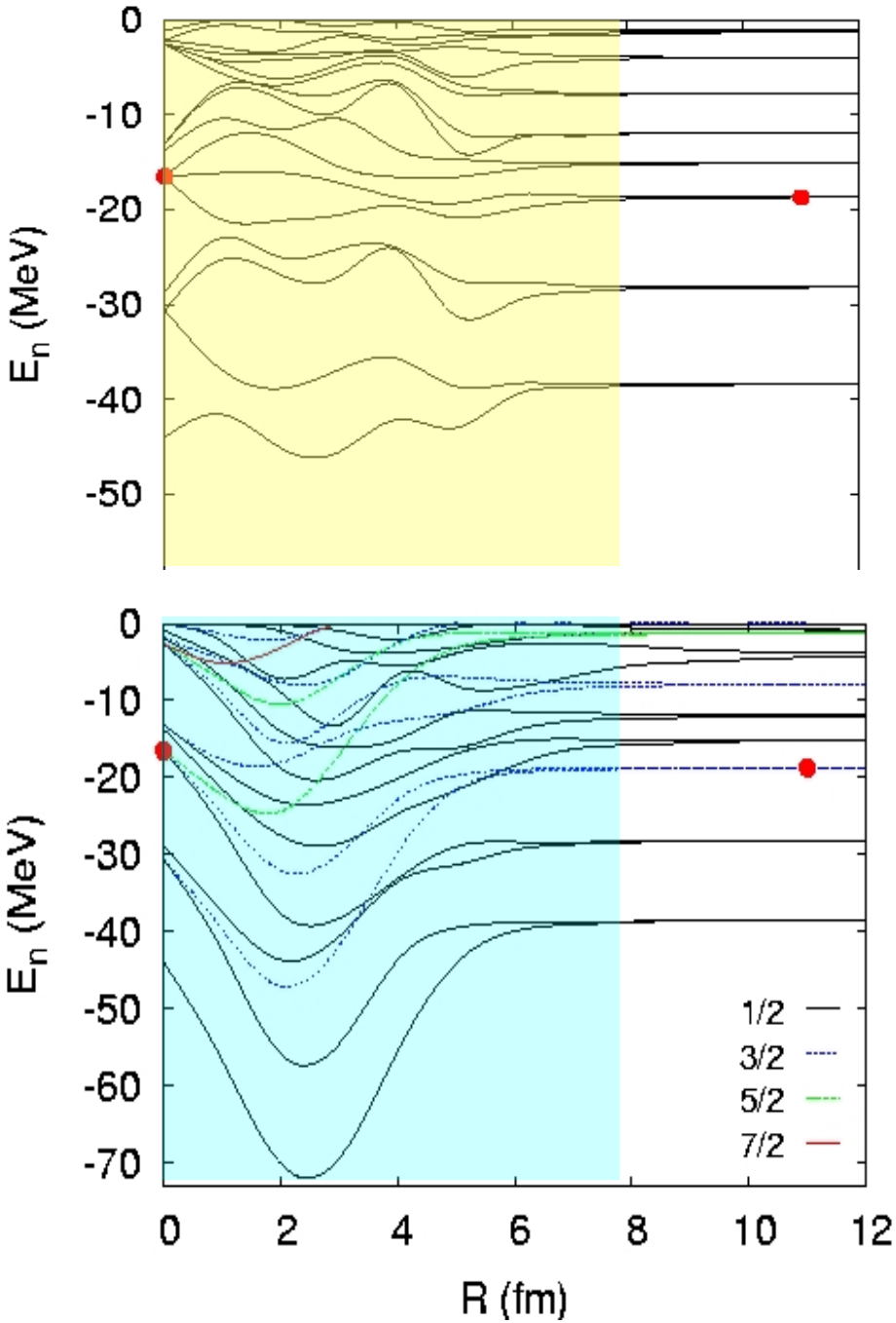
E. Uegaki & Y. Abe, Prog. Theor. Phys. **90** (1993) 615

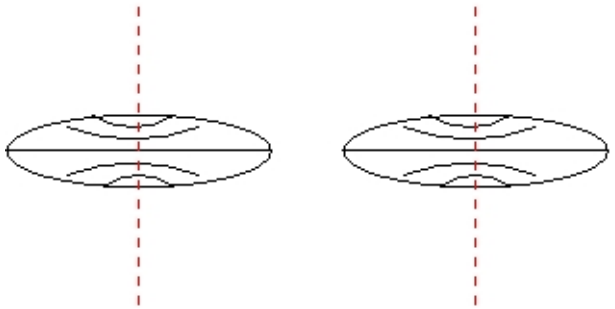
W. Greiner, J.Y. Park & W. Scheid, in Nuclear Molecules, World Scientific, 1994



How does this di-nuclear structure affect low-energy fusion?

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





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

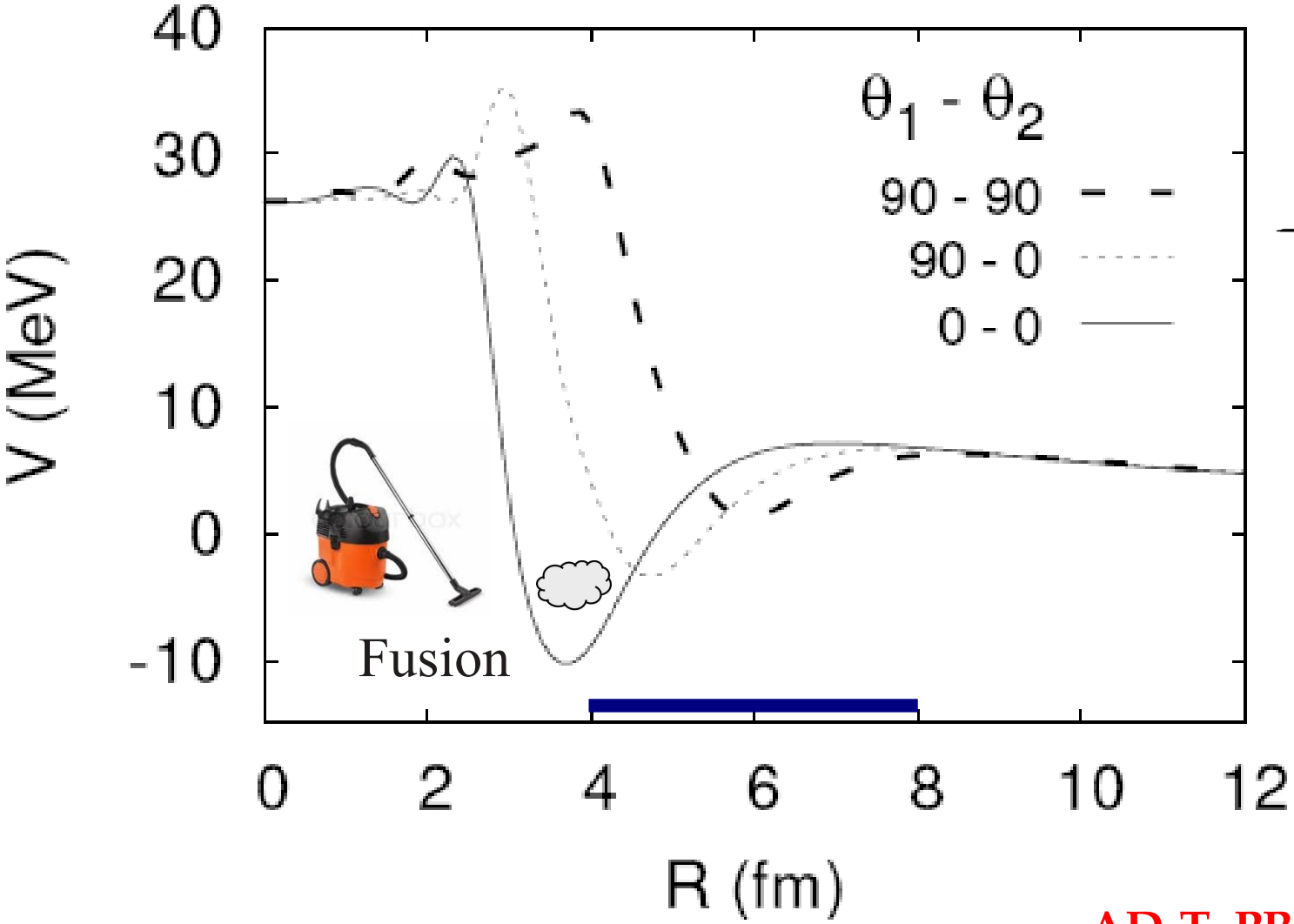
$$V_s \approx \sum_{\nu\mu}^{N} |s\nu\rangle\, V^s_{\nu\mu}\, \langle s\mu|$$

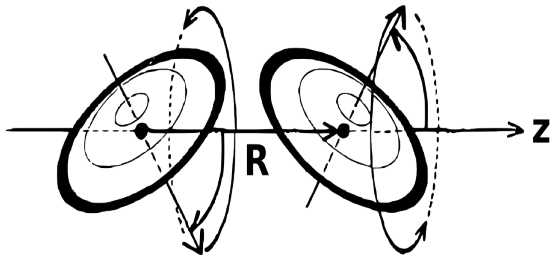
Potential Separable Expansion Method

AD-T, PRL 101 (2008) 122501

Quantum Partner-Dance of Two ^{12}C Nuclei

Collective Potential Energy Surface





AD-T, PRL 101 (2008) 122501

The dance-like movements are guided by the kinetic-energy operator.

Kinetic-energy Operator in a Mixed Representation

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

$$
\begin{aligned}
\frac{2\hat{T}}{\hbar^2} = & -\frac{1}{\mu}\frac{\partial^2}{\partial R^2} + \left(\frac{1}{I_1} + \frac{1}{\mu R^2}\right)\hat{j}_1^2 + \left(\frac{1}{I_2} + \frac{1}{\mu R^2}\right)\hat{j}_2^2 \\
& + \frac{1}{\mu R^2}\left[\hat{j}_{1,+}\hat{j}_{2,-} + \hat{j}_{1,-}\hat{j}_{2,+} + J(J+1)\right. \\
& \left. - 2k_1^2 - 2k_1k_2 - 2k_2^2\right] - \boxed{\frac{C_+(J,K)}{\mu R^2}\left(\hat{j}_{1,+} + \hat{j}_{2,+}\right)} \\
& - \boxed{\frac{C_-(J,K)}{\mu R^2}\left(\hat{j}_{1,-} + \hat{j}_{2,-}\right)}
\end{aligned}
$$

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 $k_i \rightarrow k_i \pm 1$.

Time-dependent wave-packet dynamics

- The definition of the initial state $\Psi(t=0)$.

- The time propagation, $\Psi(0) \rightarrow \Psi(t)$, guided by the evolution operator, $exp(-i\,\hat{H}\,t/\hbar)$, where $\hat{H}$ is the total Hamiltonian.

- The calculation of the **fusion cross section** from the time-dependent wave function.

Initial Wave Function: the ^{12}C nuclei are far apart

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

Radial motion

Internal motion

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

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

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

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

Evolution operator

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

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

Energy-resolved Transmission Coefficients

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

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

Method 1

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

$$\mathcal{P}(E_k) = \langle \Psi | \hat{\Delta} | \Psi \rangle$$

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

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

Energy-resolved Transmission Coefficients

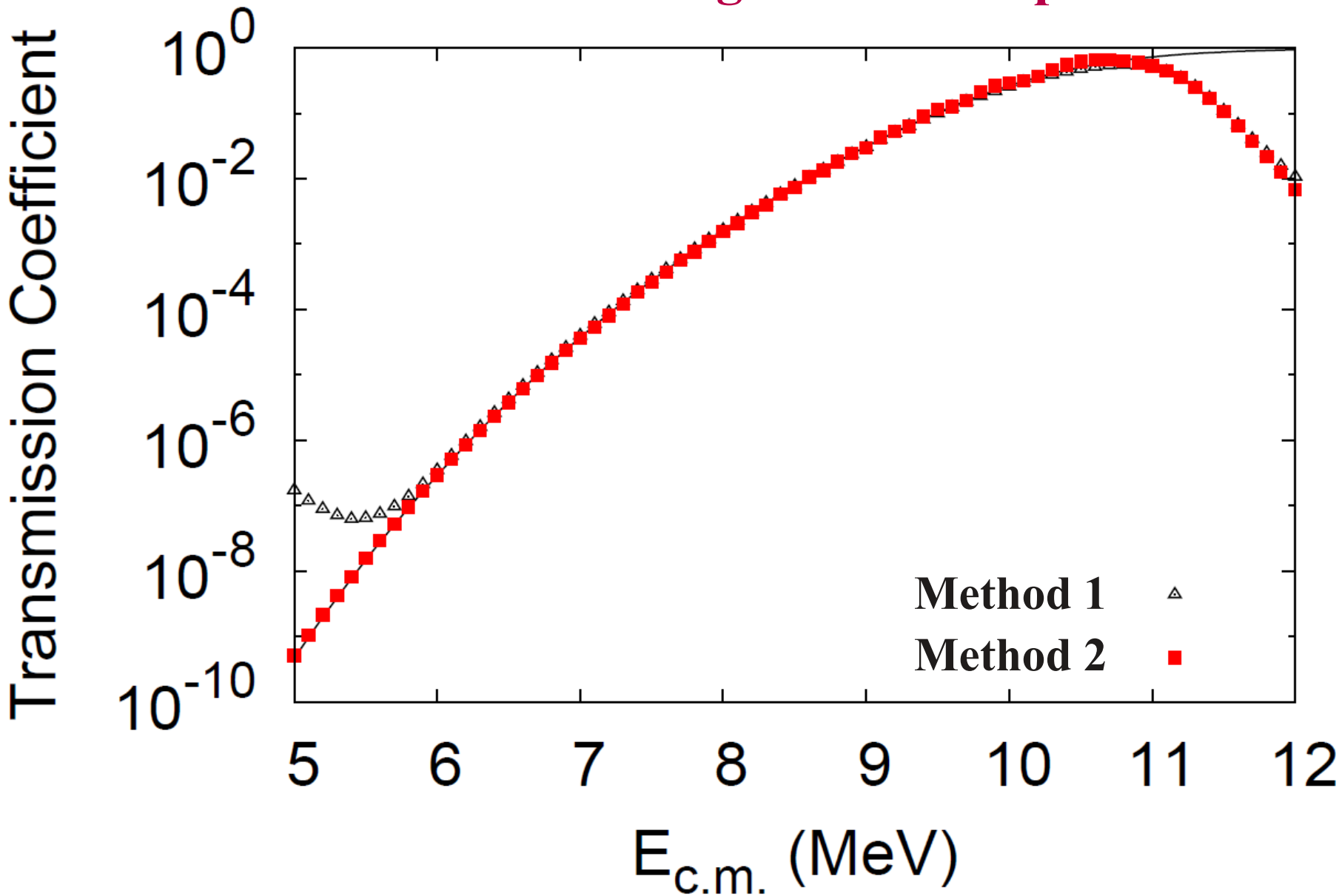
Method 2

Absorption Potential

$$T(E_k) = \frac{-(8/\hbar v_k)\,\langle \Psi | \mathrm{Img}(\hat{W})\hat{\Delta} | \Psi \rangle}{\mathcal{P}^{initial}(E_k)}$$

Time-dependent wave-packet method for $^{16}O+^{16}O$

For L=0 & Broglia-Winther potential

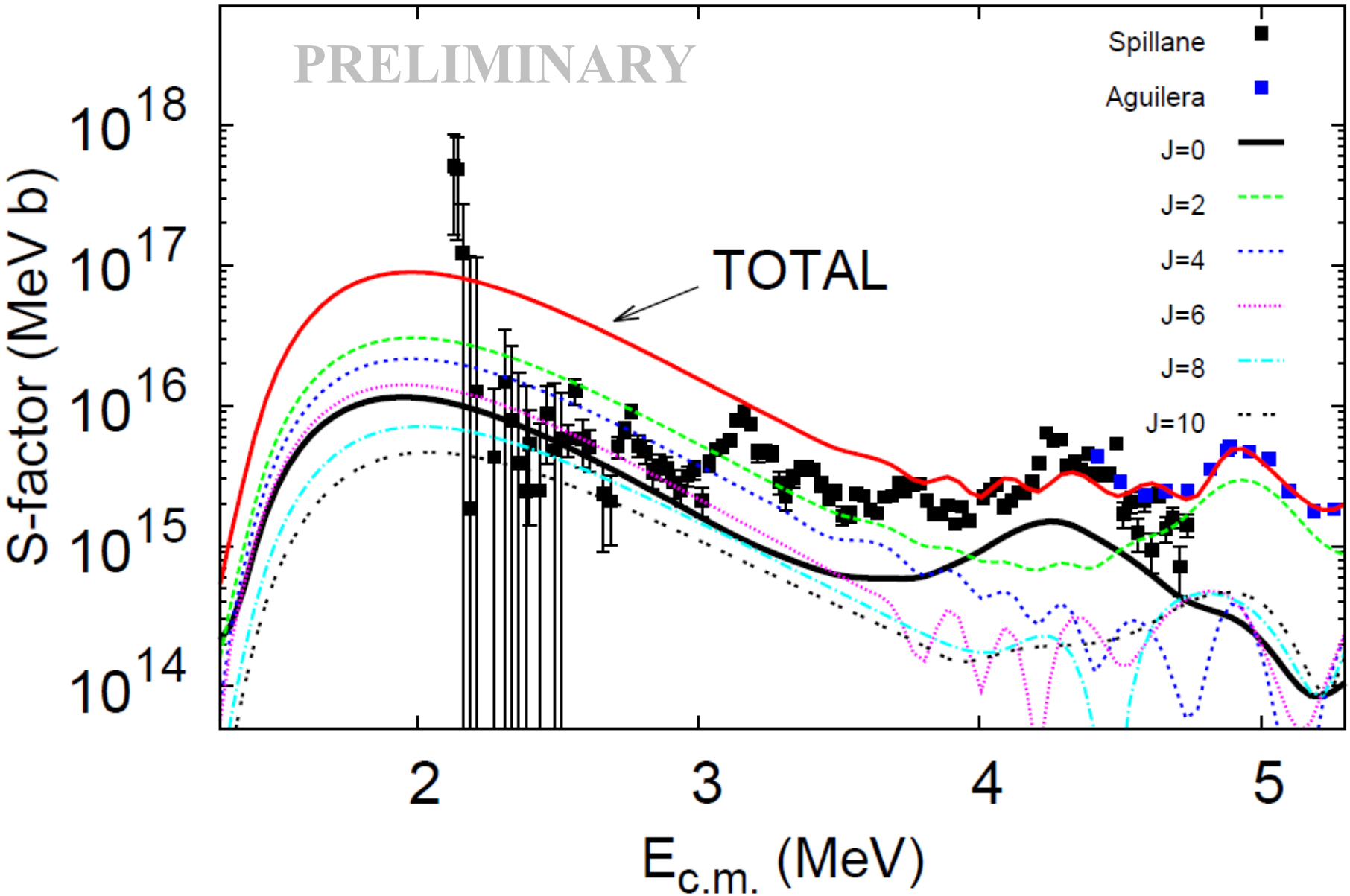


Fusion Cross Section

$$\sigma(E) = \frac{\pi\hbar^2}{\mu E} \sum_{even\ J} (2J+1)\ T_J(E)$$

Transmission Coefficient

S-Factor Excitation Curve for $^{12}C + ^{12}C$



Molecular structure & fusion are closely connected.

What I told you

- Dynamical quantum model of heavy-ion fusion within a nuclear molecular picture.

  Time-dependent wave-packet dynamics.

- Generated sub-Coulomb fusion resonances seem to correspond well with observations.

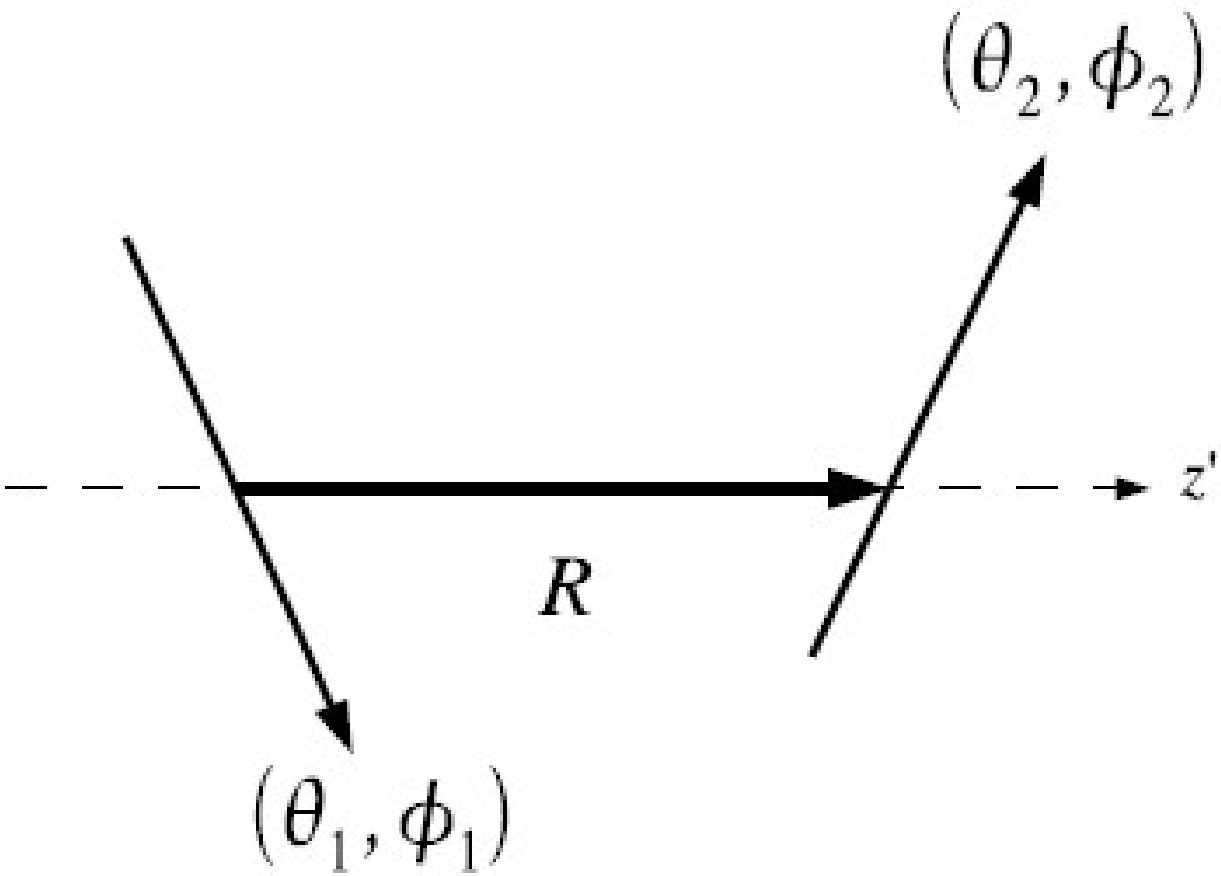
  Molecular structure & fusion are closely connected.

- Suitable tool for expanding the cross section predictions towards lower energies.

EXTRA SLIDES

Quantum Partner-Dance of Two ^{12}C Nuclei

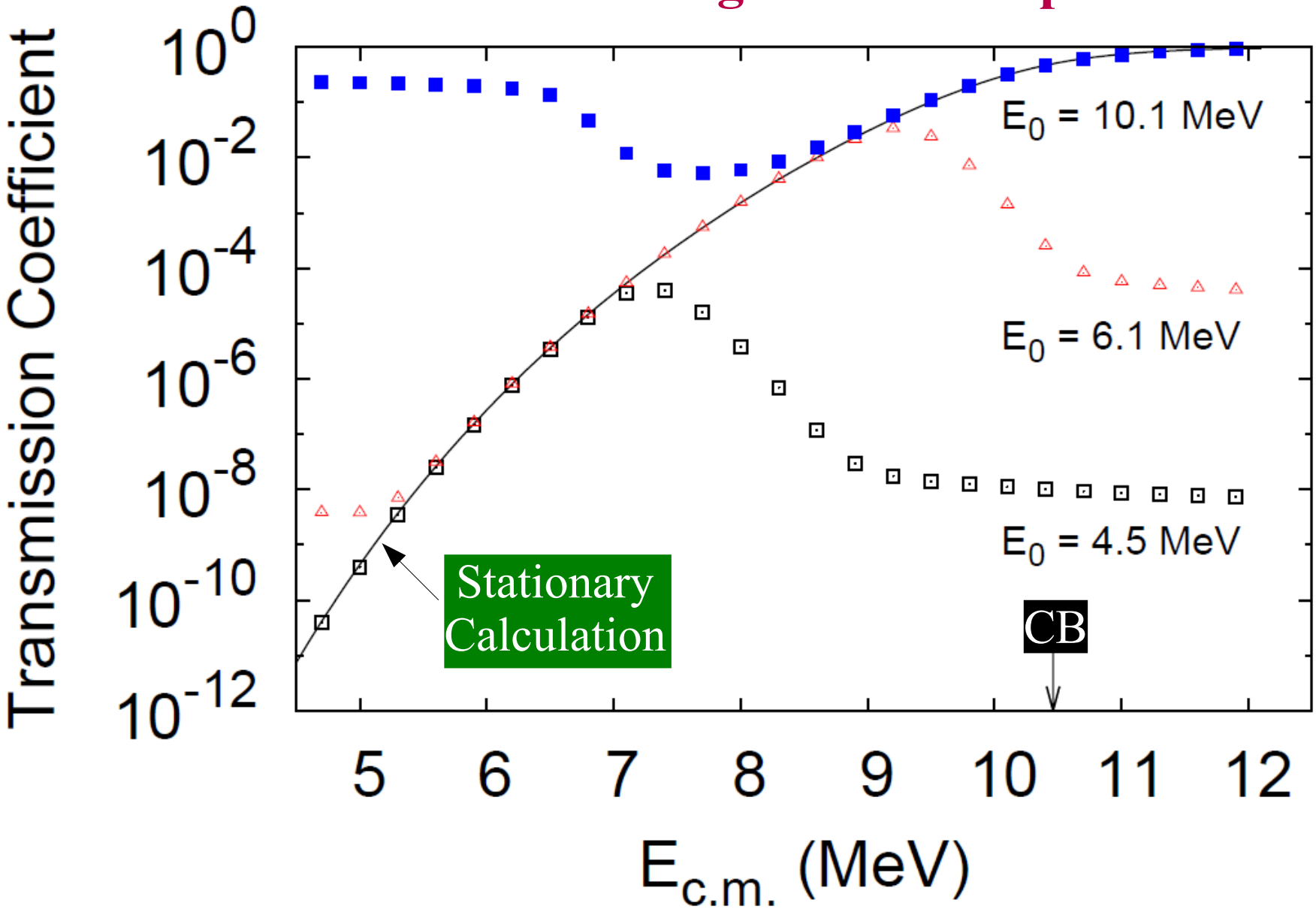
Collective Coordinates in the Rotating C.M. Frame



AD-T & Wiescher, J. of Phys.: Conf. Series 492 (2014) 012006

Time-dependent wave-packet method for $^{16}O+^{16}O$

For L=0 & Broglia-Winther potential



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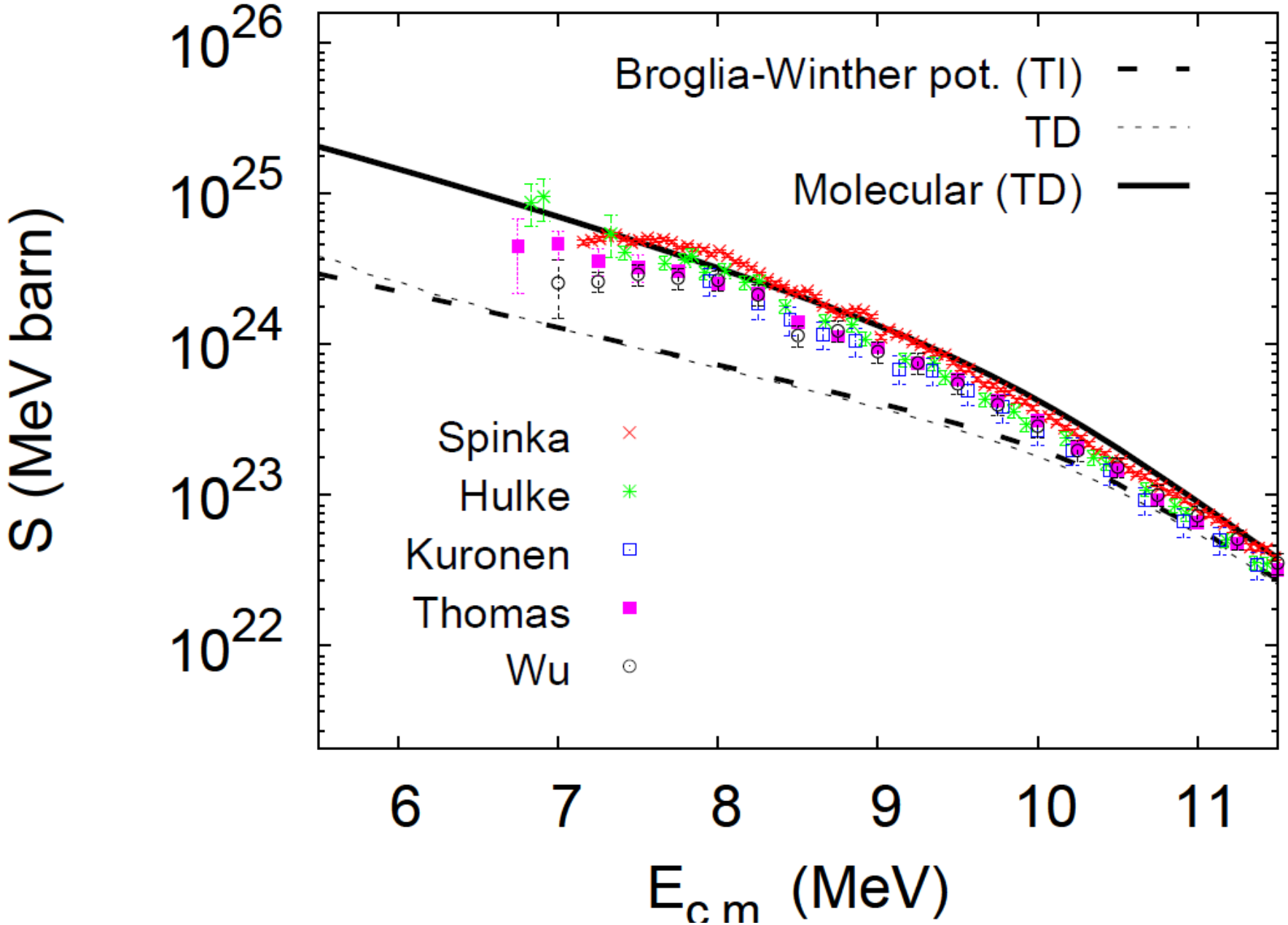
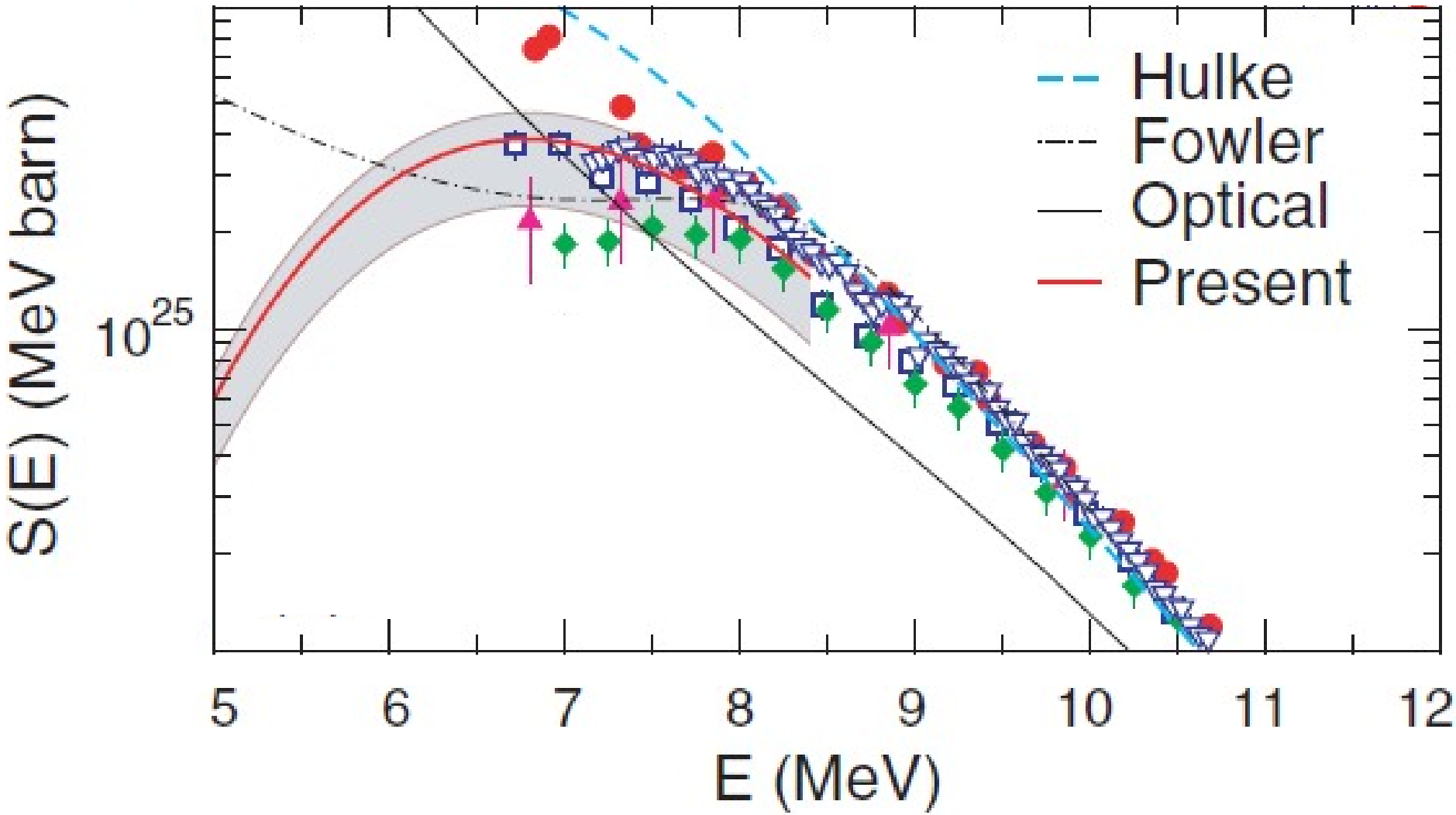
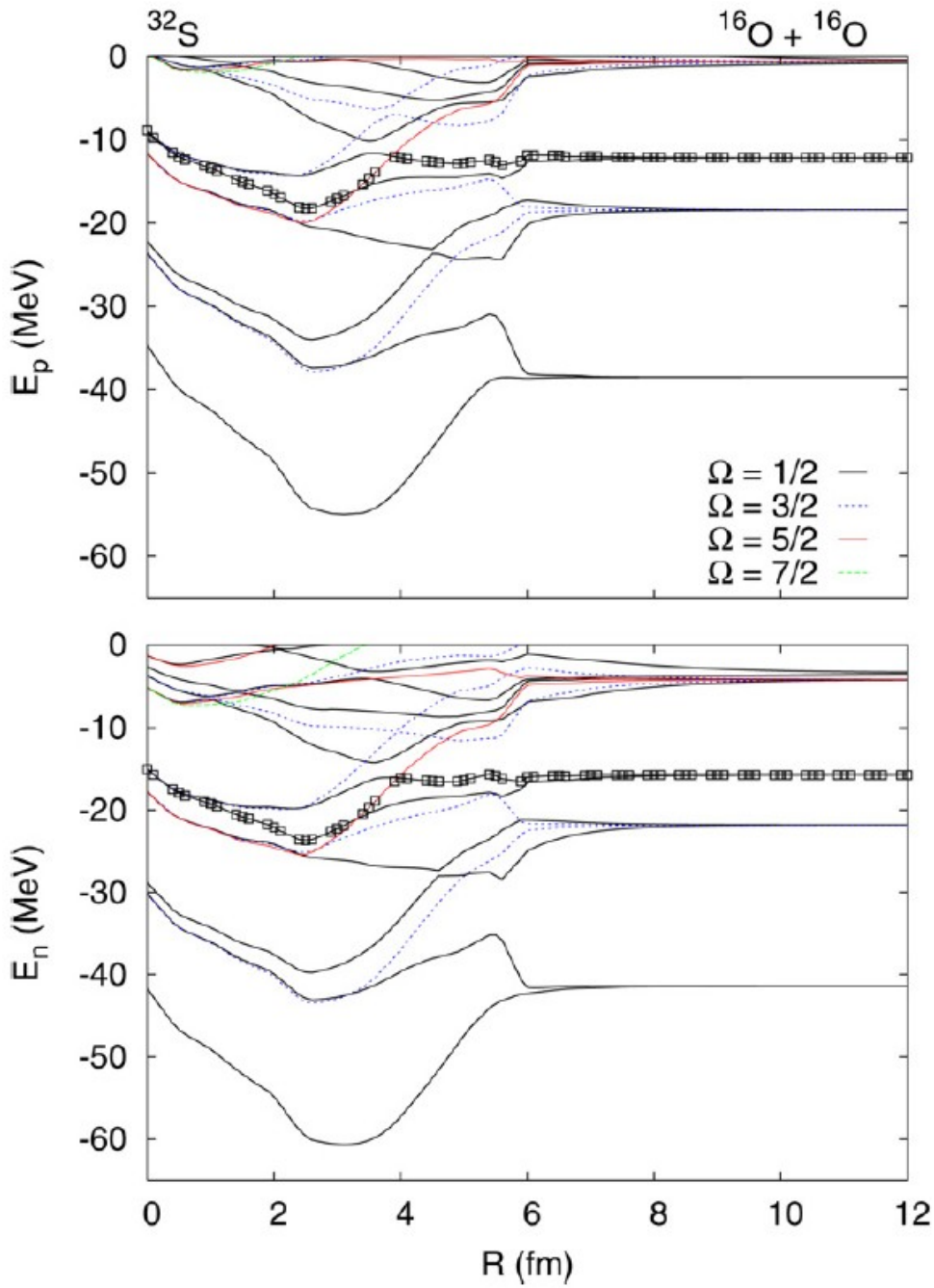


S-Factor Excitation Curve for $^{16}O + ^{16}O$

C.L. Jiang et al., Phys. Rev. C **75** (2007) 015803



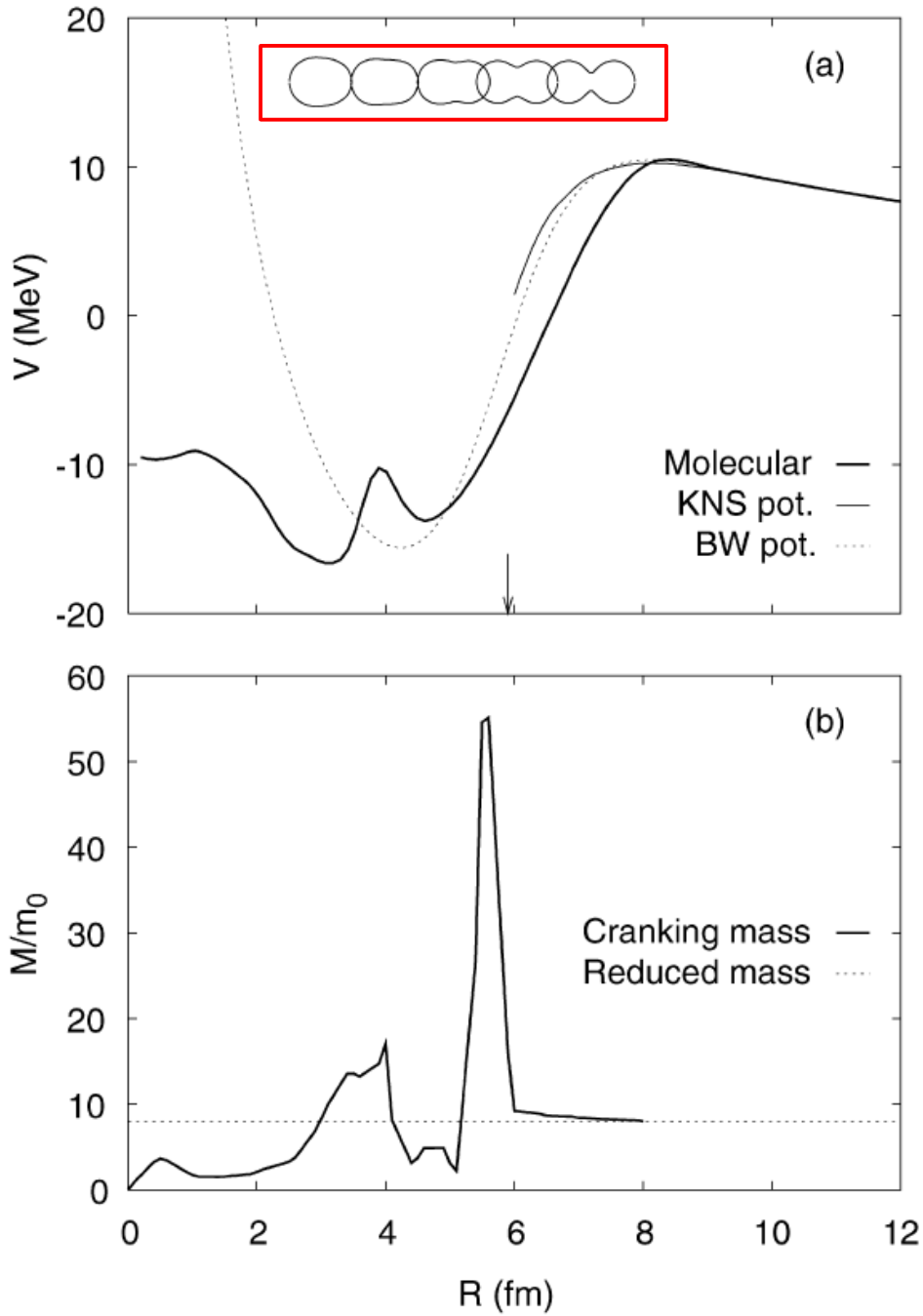
Two-Center Shell Model: $^{32}S \longrightarrow {}^{16}O + {}^{16}O$



AD-T & Scheid,

NPHA 757 (2005) 373

Collective Potential & Mass Parameter: $^{16}O + ^{16}O$



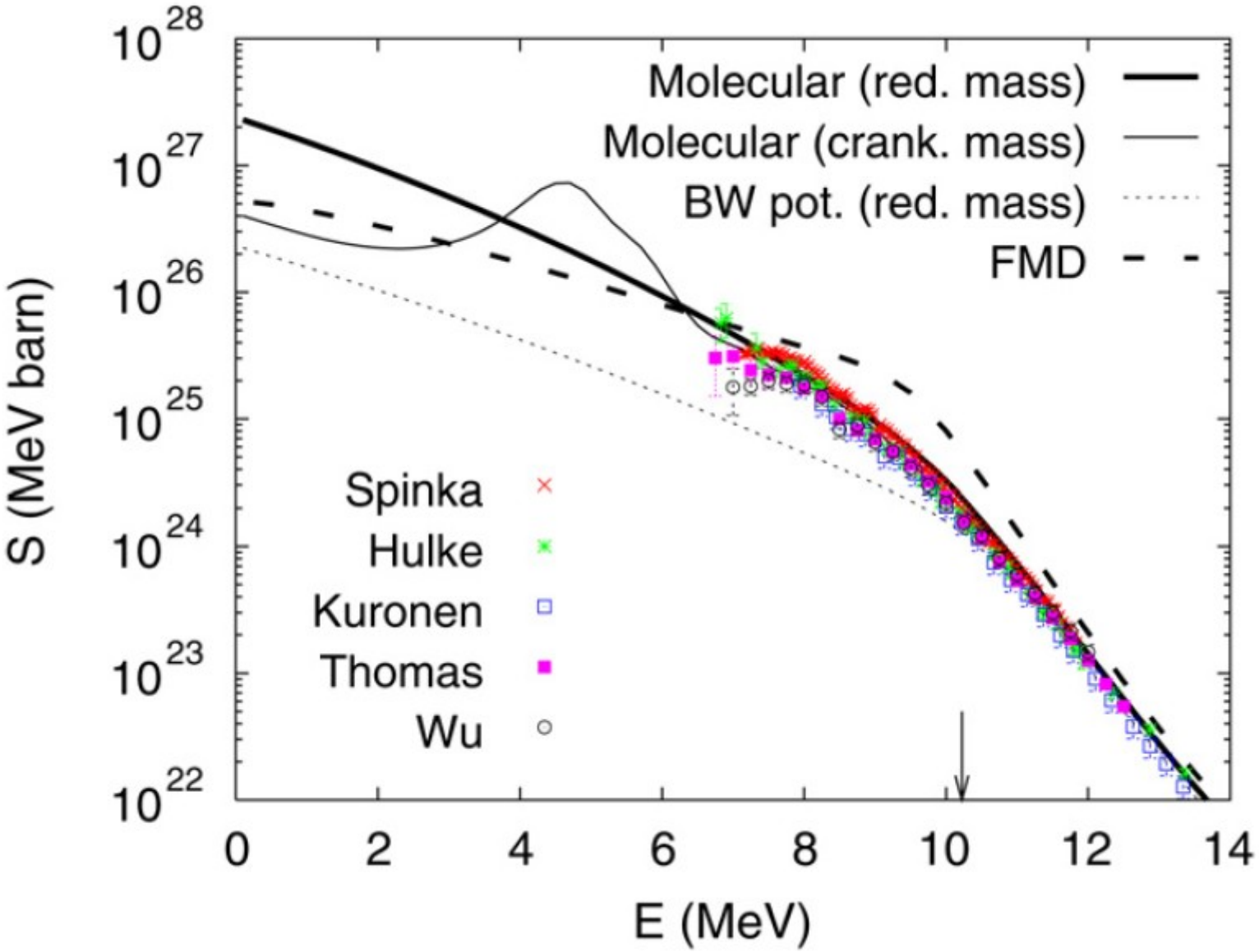
AD-T, Gasques & Wiescher,

PLB 652 (2007) 255

$$M(R) = 2\hbar^2 \sum_{i=1}^{A} \sum_{j>A} \frac{|\langle j|\partial/\partial R|i\rangle|^2}{E_j - E_i}$$

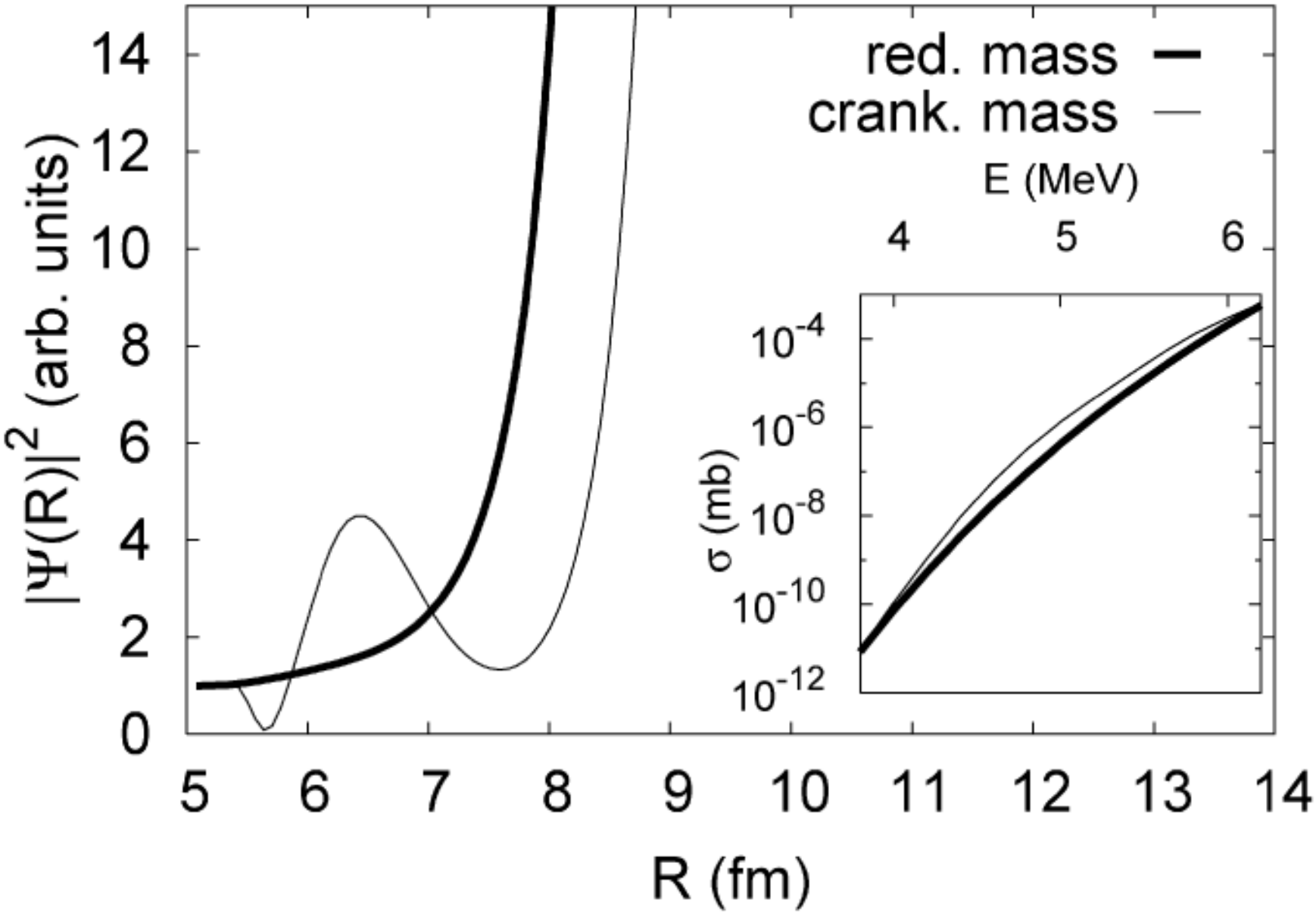
S-Factor Excitation Curve for $^{16}O+^{16}O$

AD-T, Gasques & Wiescher, PLB 652 (2007) 255



Probability distribution of the s-wave for $^{16}O+^{16}O$

AD-T, Gasques & Wiescher, PLB 652 (2007) 255



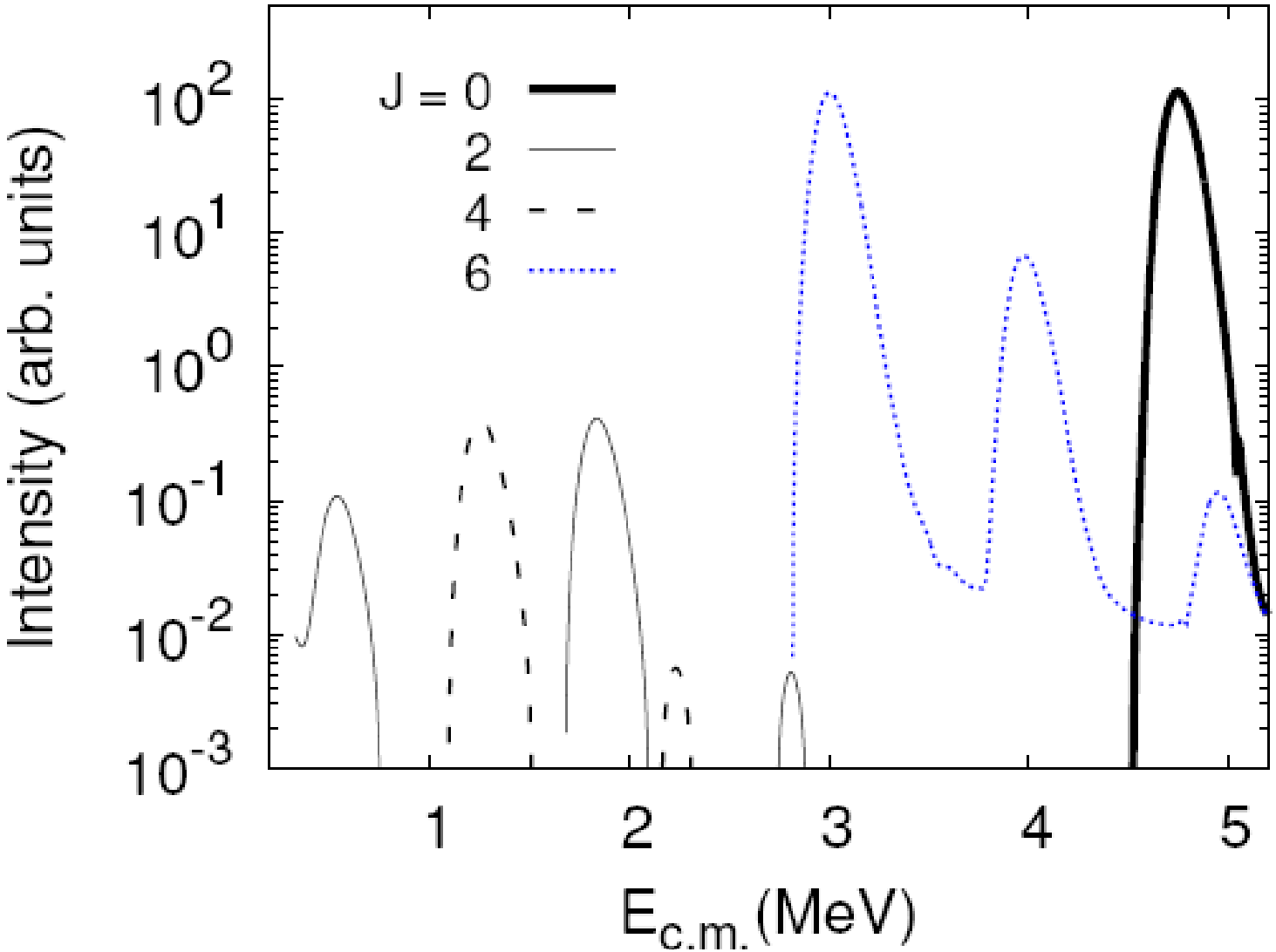
Molecular Collective States

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

$$C_J(t) = \langle \Psi_J(0) | \Psi_J(t) \rangle$$

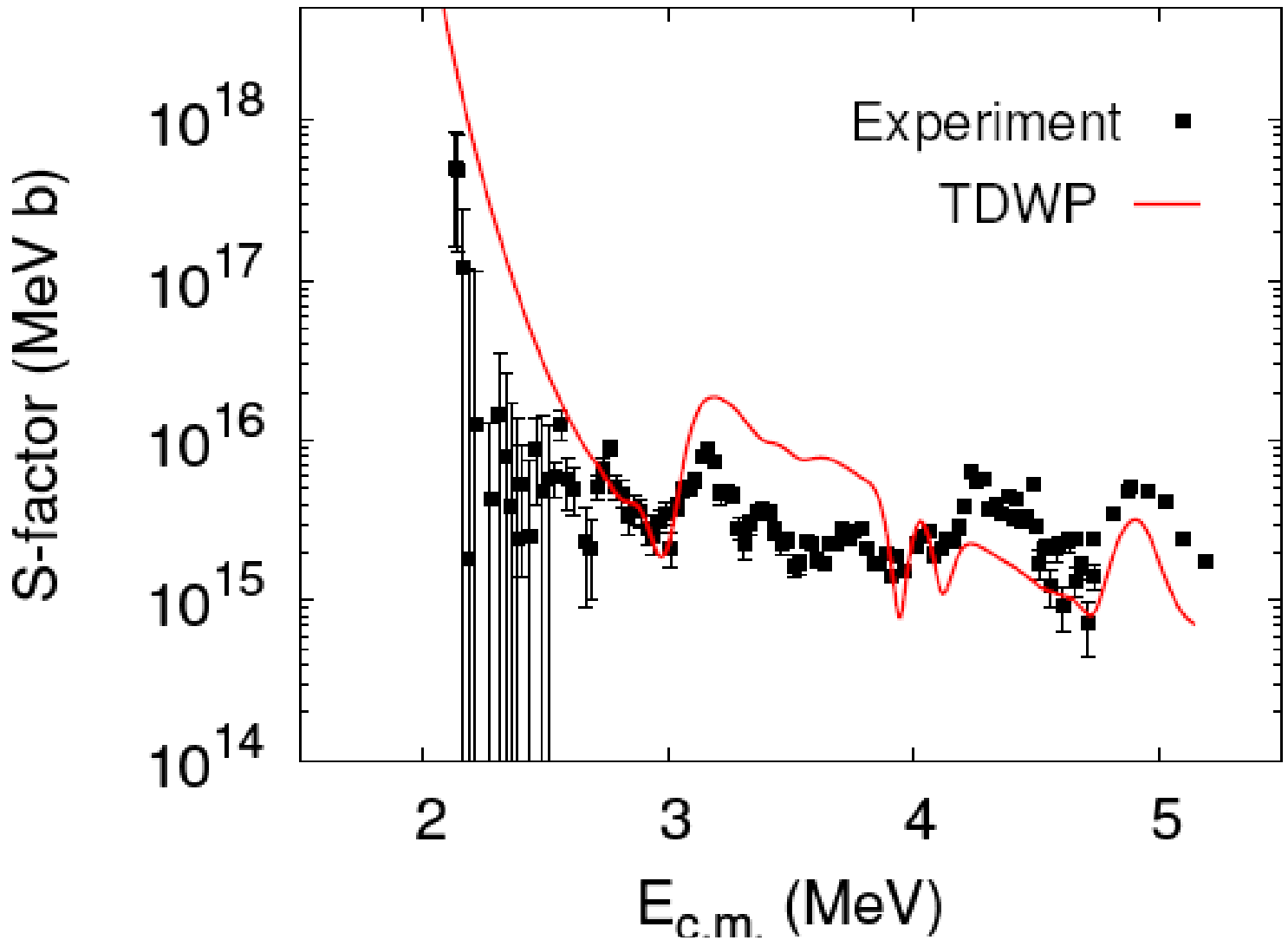
The time-to-energy Fourier Transform provides molecular collective states.

Molecular Collective States



Widths (~ 100 keV) relates to lifetime of the DNS in the potential pockets.

S-factor Excitation Function



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