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

ALEXIS DIAZ-TORRES

Examples

- $^6\text{Li} + ^{209}\text{Bi}$
- $^{12}\text{C} + ^{12}\text{C}$
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:** $\Psi(0) \rightarrow \Psi(t)$, 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

\[
H = \frac{P_{x_{CM}}^2}{2M_{T12}} + \frac{P_{\xi}^2}{2m_{12}} + U_{12}(\xi) + V_{T1}(x_{CM} - a\xi) + V_{T2}(x_{CM} + b\xi)
\]

\[
x_1 = x_{CM} - a\xi
\]

\[
x_2 = x_{CM} + b\xi
\]
To simulate fusion (irreversibility): acting inside the Coulomb barrier

\[ -iW_{T1}(x_1) \quad \& \quad -iW_{T2}(x_2) \]
Preparing the Initial State

\[ ^4\text{He} \quad ^2\text{H} \]

\[ \xi \text{ (fm)} \]

\[ ^6\text{Li} \]

Initial Probability Map \((^{209}\text{Bi} - ^6\text{Li})\)
Time Propagation


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

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

\[ \hat{H}_{\text{norm}} = \frac{\left( \hat{H} \hat{1} - \hat{H} \right)}{\Delta H} \]

The Chebyshev Propagator

\[ a_n = i^n (2 - \delta_{n0}) \exp \left( -i \frac{\hat{H} \Delta t}{\hbar} \right) J_n \left( \frac{\Delta H \Delta t}{\hbar} \right) \]

**Diagram:**

- **t = 13 \times 10^{-22} \text{ s}**
- **t = 20 \times 10^{-22} \text{ s}**
♦ Projection operator acting on the position $x_i$ of the fragment relative to the target (Heaviside function)

$$P_i = \Theta(R_{bi} - x_i)$$

$$Q_i = 1 - P_i$$

♦ Act with $(P_1 + Q_1)(P_2 + Q_2) = 1$ on the wave function:

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

<table>
<thead>
<tr>
<th>CAPTURED</th>
<th>NON CAPTURED</th>
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<tbody>
<tr>
<td>CF</td>
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<td>ICF</td>
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Potential: $^{209}$Bi - $^4$He
Energy spectra of $\Psi(t)$ as expectation values of the window operator

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

\[ E_{k+1} = E_k + 2\epsilon \]

\[ \mathcal{P}(E_k) = \langle \Psi | \hat{\Delta} | \Psi \rangle, \text{ for instance, } n = 2 : \]

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

\[ \mathcal{P}(E_k) = \langle \chi_k | \chi_k \rangle \]
Results

Energy-resolved total transmission coefficient for different values of mean energy of the initial wave packet $\sigma_0 = 10$ fm and $X_0 = 120$ fm.
Summarising


- **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?

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

![Graph showing S-factor vs. E_{c.m.} (MeV) for $^{12}\text{C} + ^{12}\text{C}$ fusion with data from various sources: Spillane et al., Aguilera et al., Becker et al., High and Cujec, Mazarakis and Stephens, Patterson et al.]

- **S-factor (MeV b)**
  - $10^{15}$
  - $10^{16}$
  - $10^{17}$
  - $10^{18}$

- **E_{c.m.} (MeV)**
  - 2
  - 3
  - 4
  - 5
  - 6

- **Cross section**
  - 1 pb
  - 1 nb
Coupled-Channels Calculations for $^{12}\text{C} + ^{12}\text{C}$

Jiang, Esbensen et al., PRL 110 (2013) 072701
THINK OUTSIDE THE BOX

XOX
XXX
XOX

OXX
OXO
The $^{12}\text{C} + ^{12}\text{C}$ Molecular Structure
Greiner, Park & Scheid, in Nuclear Molecules, World Scientific, 1994

Quadrupole deformation of $^{12}\text{C}$: $\sim -0.5$

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

\[ J = 0 \]

Transmission Coefficient

\[ \log_{10}(T) \]

\[ E_{\text{c.m.}} \text{ (MeV)} \]

- \( R_0 = 3.7 \text{ fm} \)
- \( R_0 = 6.0 \text{ fm} \)
Phase shift analysis of effective potentials for $^{12}\text{C} + ^{12}\text{C}$
Astrophysical S-Factor for $^{12}\text{C} + ^{12}\text{C}$ Fusion

![Graph showing the S-factor (MeV b) vs. E_c.m. (MeV) for different experiments and theoretical models.](image-url)
Summarising


- 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

16O + 154Sm, CRC (up to $4^+$), $J=30$
Sensitivity of Molecular Shell Structure to the $^{12}$C Alignment

$$V = \sum_{s=1}^{2} e^{-iR_s \hat{k}} \hat{U}(\Omega_s) V_s \hat{U}^{-1}(\Omega_s) e^{iR_s \hat{k}}$$

$$V_s \approx \sum_{\nu \mu} \langle s\nu | V^{s}_{\nu\mu} | s\mu \rangle$$

Potential Separable Expansion Method

AD-T, PRL 101 (2008) 122501
• Energy-resolved **total transmission** for different values of the spatial width of the initial wave packet.

\[
E_0 = 28 \text{ MeV} \\
X_0 = 120 \text{ fm}
\]

![Graph showing energy resolved total transmission](image)
Energy Projection of the Wave Function

Schafer & Kulander, PRA 42 (1990) 5794

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

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

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

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

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

$P(E_k) = \langle \chi_k | \chi_k \rangle$
Results

- Energy-resolved total transmission for different values of the mean energy of the initial wave packet.
Coupled-Channels Calculations for $^{12}\text{C} + ^{12}\text{C}$

Assuncao & Descouvemont, PLB 723 (2013) 355
Fusion Cross Section & Astrophysical S-Factor

\[ S(E) = \sigma(E) E \exp \left( 2\pi \eta \right) \]

- **Structural factor** [MeV barn]
- **Fusion cross section** [barn = $10^{-28}$ m$^2$]

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

Sommerfeld parameter

\( S(E) \) represents the fusion cross section free of Coulomb suppression, which is adequate for extrapolation towards stellar energies.
\[
\frac{2 \hat{T}}{\hbar^2} = -\frac{1}{\mu} \frac{\partial^2}{\partial R^2} + \left( \frac{1}{I_1} + \frac{1}{\mu R^2} \right) \hat{j}_1^2 + \left( \frac{1}{I_2} + \frac{1}{\mu R^2} \right) \hat{j}_2^2
\]

\[+ \frac{1}{\mu R^2} \left[ \hat{j}_{1,+} \hat{j}_{2,-} + \hat{j}_{1,-} \hat{j}_{2,+} + J(J + 1) \right. \]

\[\left. - 2k_1^2 - 2k_1 k_2 - 2k_2^2 \right] - \frac{C_+(J, K)}{\mu R^2} (\hat{j}_{1,+} + \hat{j}_{2,+}) \]

\[- \frac{C_-(J, K)}{\mu R^2} (\hat{j}_{1,-} + \hat{j}_{2,-}) \]

Coriolis interaction

\(\mu\) is the reduced mass for the radial motion,

\(I_i\) is the \(^{12}\text{C}\) 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 \(k_i \to k_i \pm 1\).
Initial state $\Psi(t = 0)$: the $^{12}\text{C}$ 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

$$
\chi_0(R) = (\sqrt{\pi} \sigma)^{-1/2} \exp\left[-\frac{(R - R_0)^2}{2\sigma^2}\right] e^{i P_0(R - R_0)},
$$

Internal rotational motion

$$
\psi_0(\theta_1, k_1, \theta_2, k_2) = \left[ \zeta_{j_1, m_1}(\theta_1, k_1) \zeta_{j_2, m_2}(\theta_2, k_2) \\
+ (-1)^J \zeta_{j_2, -m_2}(\theta_1, k_1) \zeta_{j_1, -m_1}(\theta_2, k_2) \right] \\
/ \sqrt{2 + 2 \delta_{j_1, j_2} \delta_{m_1, -m_2}},
$$

where $\zeta_{j, m}(\theta, k) = \sqrt{(2j+1)(j-m)!/2 (j+m)!} \ P_j^m(\cos \theta) \delta_{km}$,  
and $P_j^m$ are associated Legendre functions.
Time Propagation of the Wave Function

\[ |\Psi_J(t)\rangle = e^{-i \frac{\hat{H} t}{\hbar}} |\Psi_J(0)\rangle \]

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

\[ \mathcal{P}(E) = \langle \Psi(t) | \delta(E - \hat{H}) | \Psi(t) \rangle \]

Energy projector

Reflection & Transmission Coefficients

\[ R(E) = \frac{\mathcal{P}_{\text{final}}(E)}{\mathcal{P}_{\text{initial}}(E)} \]

\[ T(E) = 1 - R(E) \]
Fusion Excitation Function for $^{12}$C + $^{12}$C

![Graph showing fusion excitation function for $^{12}$C + $^{12}$C]
Fusion Excitation Function for $^{12}\text{C} + ^{12}\text{C}$
Transmission coefficients for $^{16}\text{O} + ^{16}\text{O}$ central collisions
An increase in the $^{12}$C + $^{12}$C fusion rate from resonances at astrophysical energies

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