

# **Coupled-Channels Density-Matrix Approach to Nuclear Reaction Dynamics**

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# Outline

- **Introduction**
  - ✓ Quantum decoherence in a broad context
  - ✓ Coherent coupled channels model
  - ✓ Quantum decoherence in nuclear collisions
- **Coupled-channels density-matrix approach**
  - ✓ Picture and formulation
  - ✓ Applications
- **Summary**

# The Quantum to Classical transition - from coherent superposition to irreversibility

W.H. Zurek, Rev. Mod. Phys. **75** (2003) 715; Phys. Today **44** (1991) 36

M. Schlosshauer, Decoherence and the quantum to classical transition, Springer (2007)

P. Ball, Nature **453** (2008) 22

Idealized isolated  
system

Superposition of basis states  
Described by coherent Q.M.

Sub-system  
Larger system

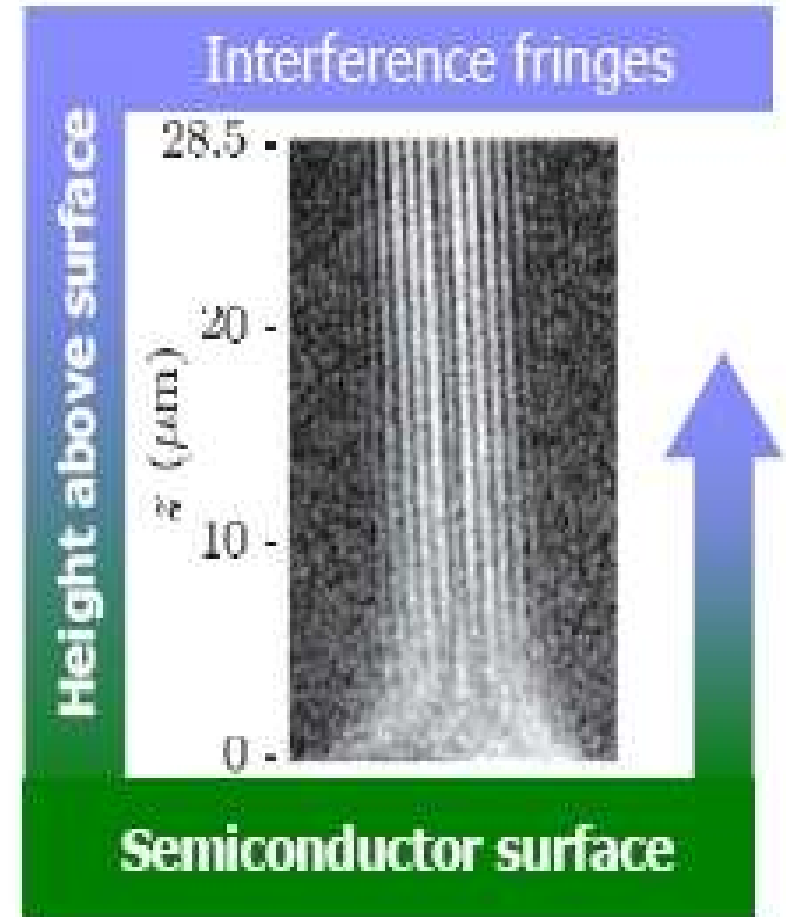
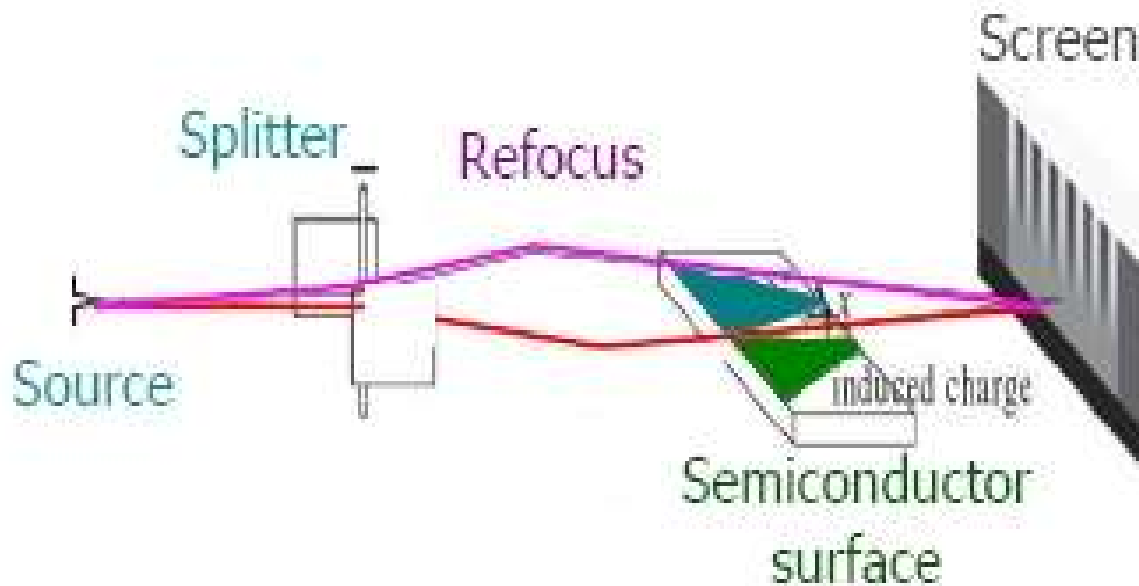
Sub-system "entangled" with environment  
Loss of coherence in smaller system  
→ Irreversible outcome (classical)  
Can be described by density matrix (Q.M.)

- Quantum decoherence – "dynamical delocalization of Q.M. superpositions"  
(H.D. Zeh arXiv:quant-ph/0512078 v2) coherence shared with (lost in) environment

# Quantum Decoherence

Example: Electron entanglement with a surface

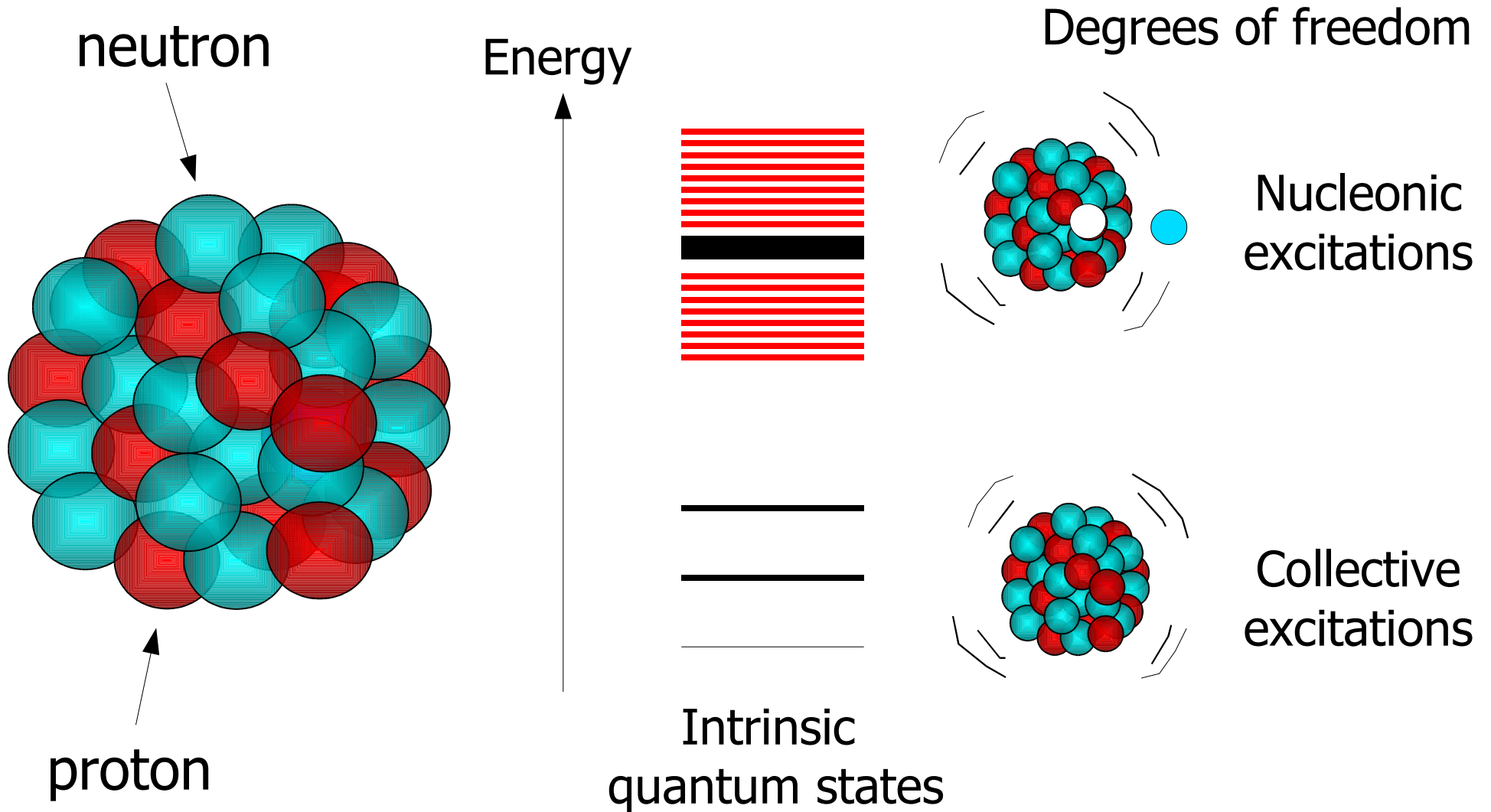
Double-slit type experiment with single electrons



P. Sonnentag et al., PRL **98** (2007) 200402

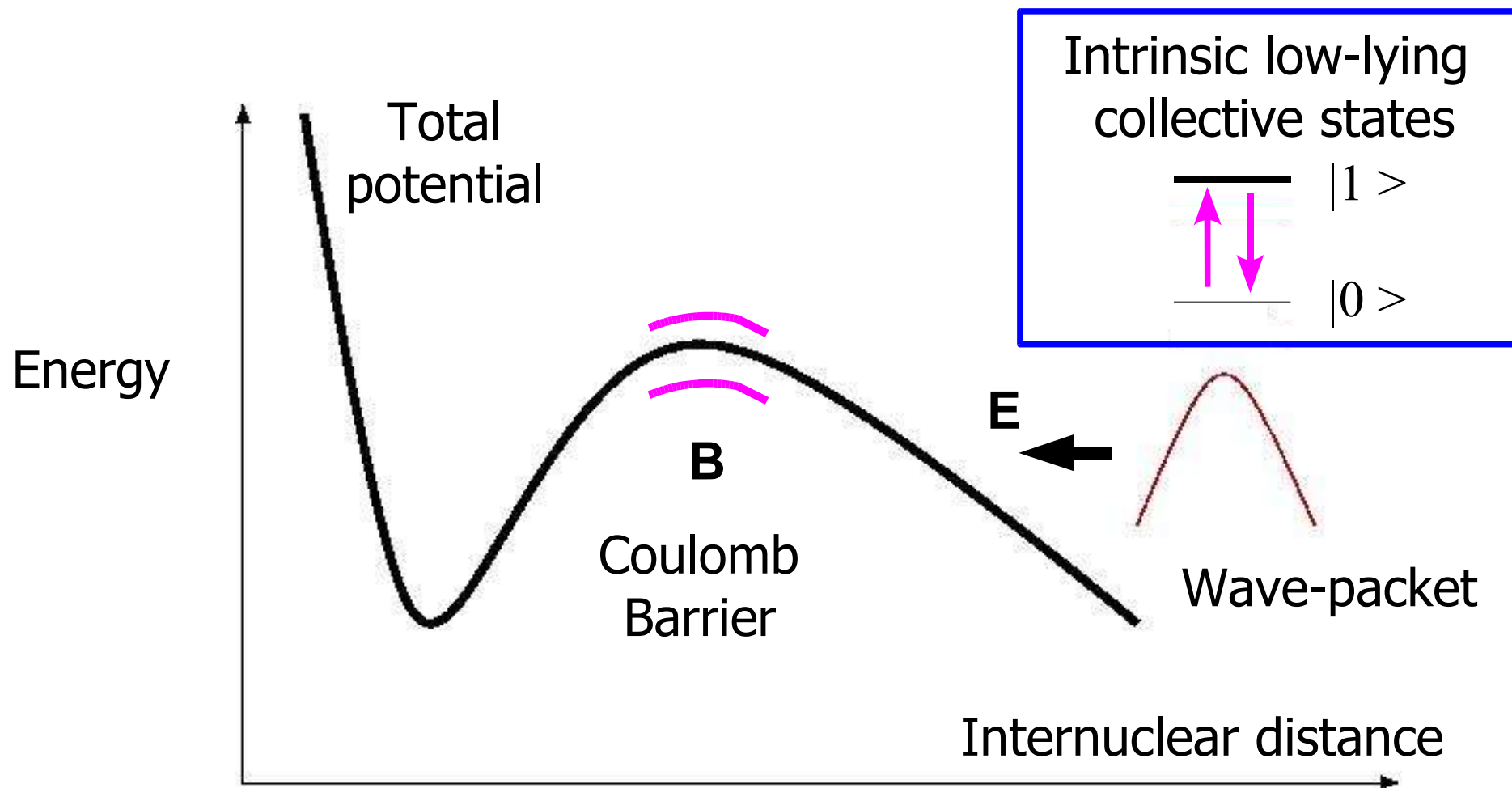
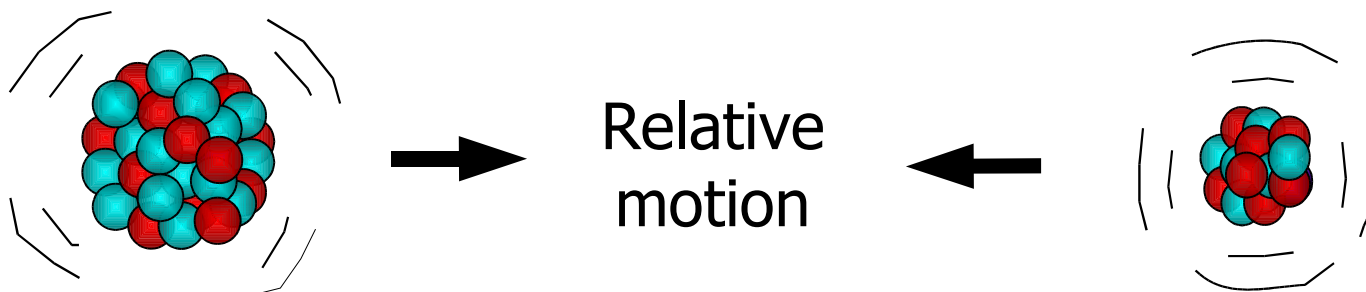
Can a quantitative model be developed for nuclear collisions ?

# Composite Atomic Nucleus



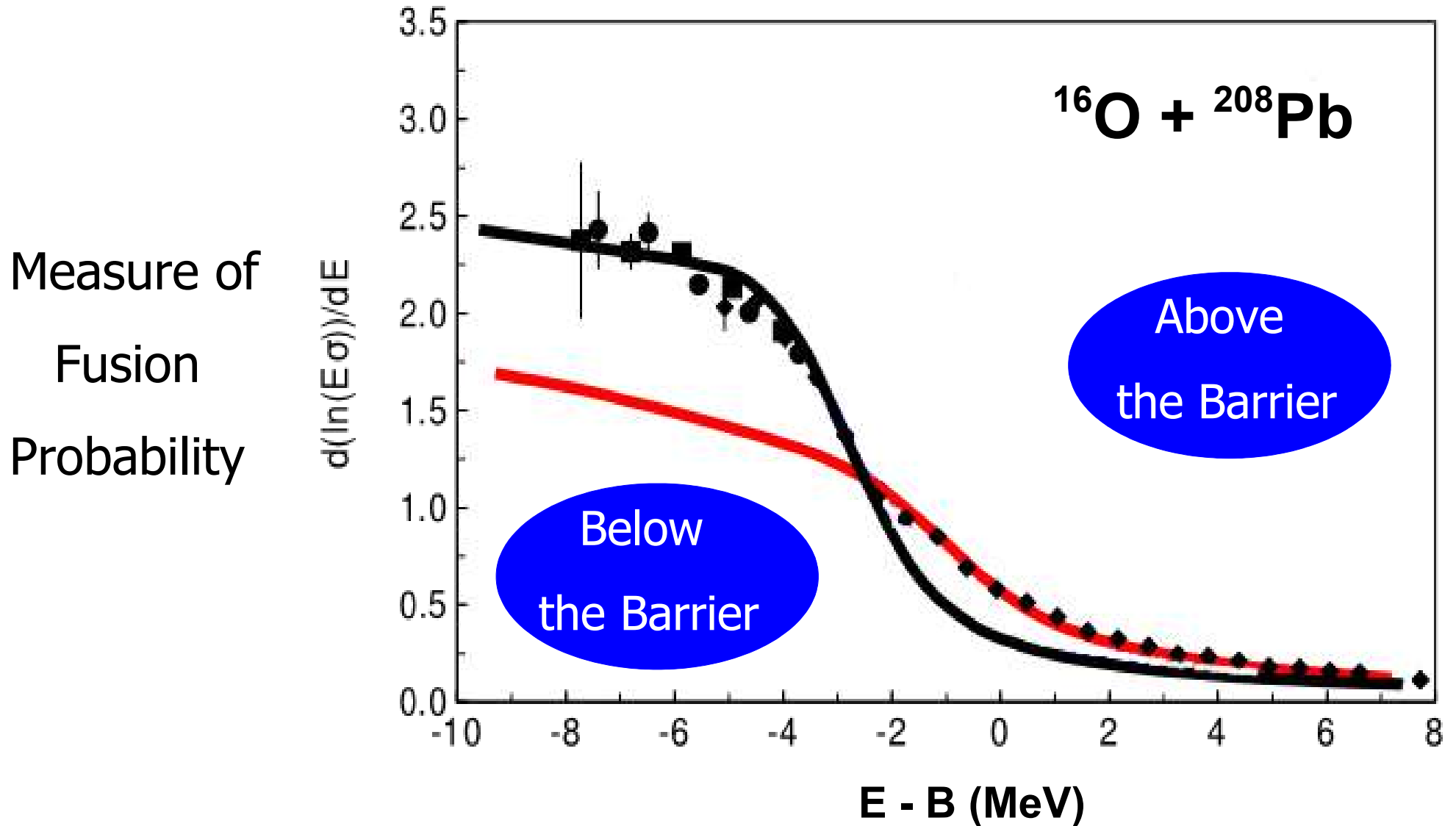
How do these excitations affect the nuclear collision dynamics ?

# Low-Energy Collision Dynamics: Coherent Quantum Description



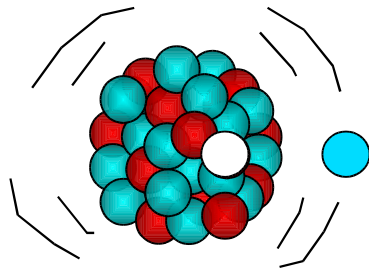
# Failure of the Coherent Quantum Description

Coupling Assisted Quantum Tunnelling: Nuclear Fusion

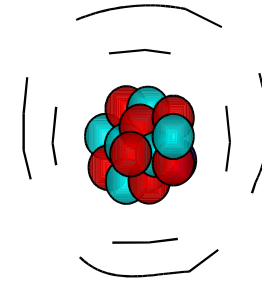


# Quantum Decoherence in Nuclear Collisions

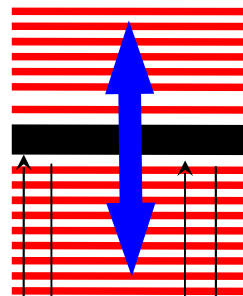
AD-T, Hinde, Dasgupta, Milburn & Tostevin, PRC 78 (2008) 064604



Relative motion

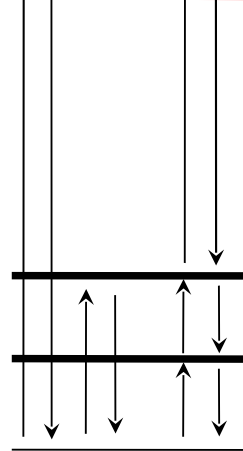


$|I_k\rangle$



$|3\rangle$

Suppresses quantum tunnelling (sub-barrier fusion)

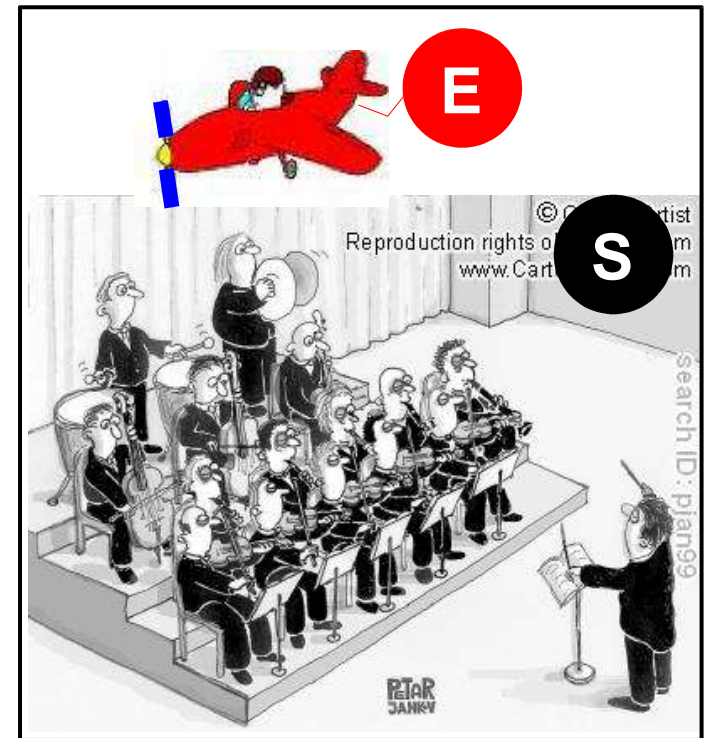


$|2\rangle$

$|1\rangle$

$|0\rangle$

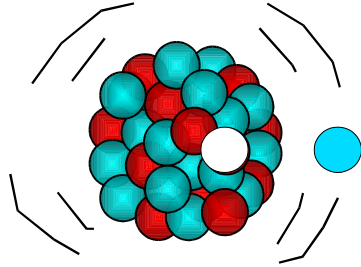
Intrinsic quantum states



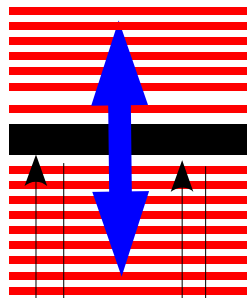


# Quantum Decoherence in Nuclear Collisions

AD-T, Hinde, Dasgupta, Milburn & Tostevin, PRC 78 (2008) 064604

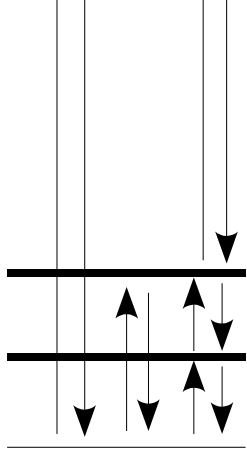


**E**



$|3\rangle$

$|I_k\rangle$



$|2\rangle$

$|1\rangle$

$|0\rangle$

**S**

Intrinsic quantum states

$$\partial \hat{\rho} / \partial t = [\hat{\mathcal{L}}_H + \hat{\mathcal{L}}_D] \hat{\rho}, \quad \hat{\rho}(0) = \hat{\rho}_0 \quad \text{Master equation}$$

$$\hat{\mathcal{L}}_H \hat{\rho} = -i[\hat{H}, \hat{\rho}] / \hbar \quad \text{Schrödinger description}$$

$$\hat{\mathcal{L}}_D \hat{\rho} = \sum_{\mathbf{k}} (\hat{c}_{\mathbf{k}} \hat{\rho} \hat{c}_{\mathbf{k}}^\dagger - \frac{1}{2} [\hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}}, \hat{\rho}]_+)$$

**Decoherence & Absorption**

$$\hat{c}_{Ij} = \sqrt{\Gamma_{Ij}} |I\rangle \langle j|$$

Example : 1- dimensional model

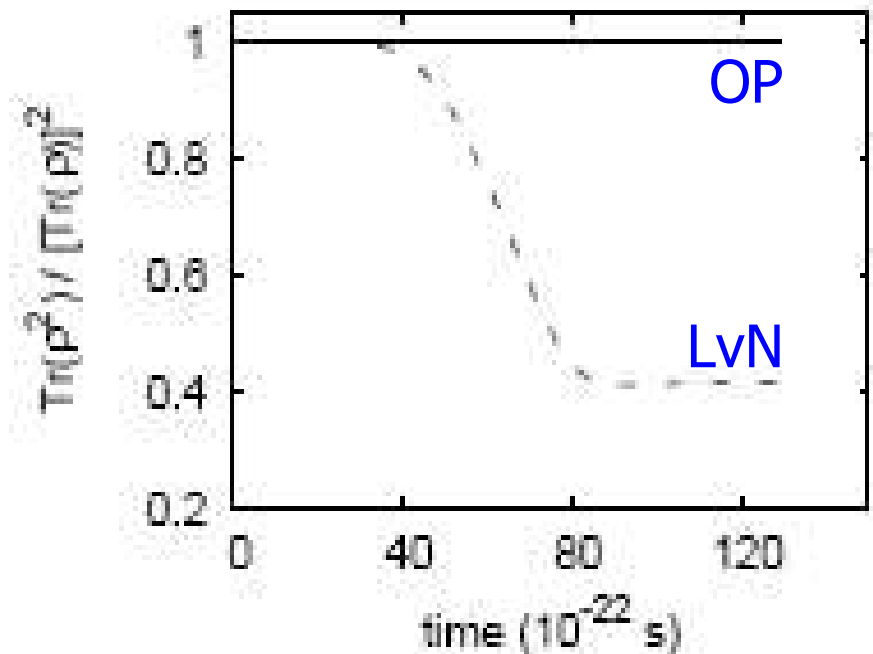
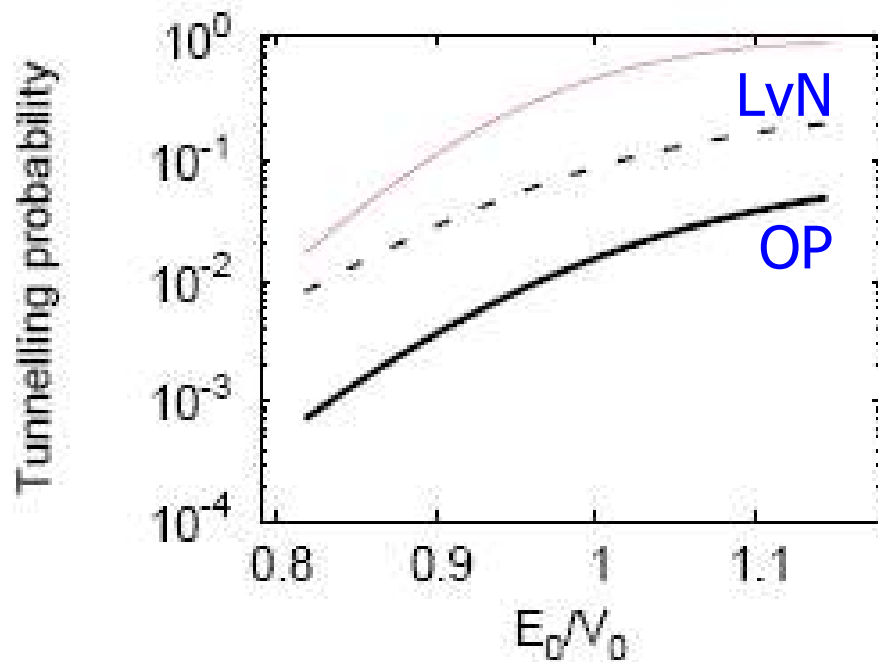
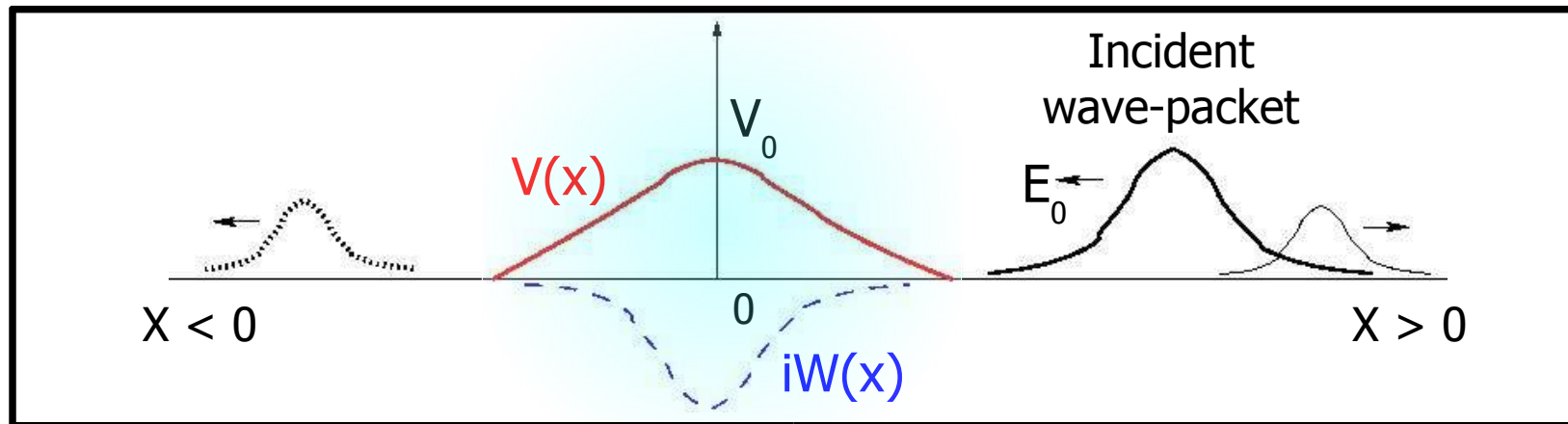
$$\hat{\rho}(t) = \sum_{ij,rs} |r\rangle |i\rangle \rho_{ij}^{rs}(t) \langle j| \langle s|, \quad \rho_{ij}^{rs}(0) = \rho_{00}^{rs}(0) = g_0(r) g_0^*(s)$$

$|i\rangle, i = 1, \dots, N$       Intrinsic (energy) basis

$|r\rangle, r = 1, \dots, M$       Coordinate (grid) basis

# Quantum Decoherence in Nuclear Collisions

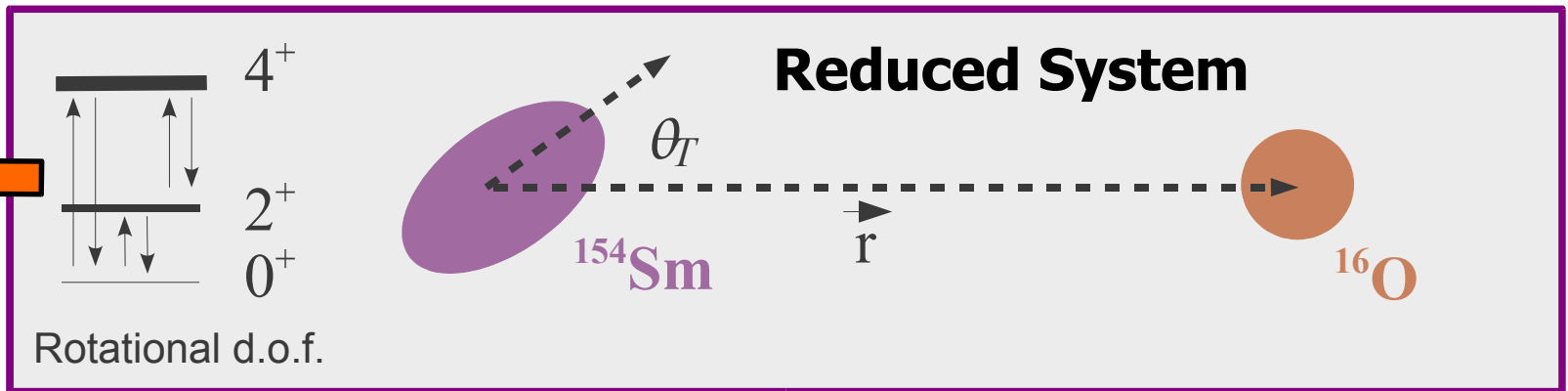
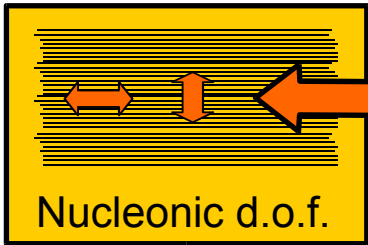
## Absence of Decoherence in the Optical Potential Model



Decoherence significantly affects quantum tunnelling, and thus scattering as well

# Coupled-Channels Density-Matrix Approach

Environment



$$|\chi\rangle = \sum_{LJM} \psi_{k_0}(\mathbf{r}) |0L; JM\rangle \Rightarrow \hat{\rho}_0 = |\chi\rangle\langle\chi|$$

$$\hat{\rho}_0 = \sum_{\alpha, \alpha', rs} |r\rangle|\alpha\rangle \rho_{\alpha\alpha'}^{rs}(t=0) \langle\alpha'|s\rangle,$$

where  $\alpha \equiv (IL; JM)$ ,  $|\alpha\rangle$  and  $|r\rangle$  are the coupled angular momentum basis and the discrete grid-basis describing the internuclear separations, respectively.

$$\rho_{\alpha\alpha'}^{rs}(t=0) = N^2 \exp\left[-\frac{(r-r_0)^2}{2\sigma^2}\right] e^{ik_0 r} \\ \times \exp\left[-\frac{(s-r_0)^2}{2\sigma^2}\right] e^{-ik_0 s} \delta_{I0} \delta_{I'0},$$

where  $N$  is determined from the normalization condition  $\sum_{r\alpha} \rho_{\alpha\alpha}^{rr} = 1$ .

# Coupled-Channels Density-Matrix Approach

## Equations of Motion

S

$$\begin{aligned} i\hbar \dot{\rho}_{\alpha\alpha'}^{rs} = & \sum_t (T^{rt} \rho_{\alpha\alpha'}^{ts} - \rho_{\alpha\alpha'}^{rt} T^{ts}) \\ & + [U_\alpha(r) - U_{\alpha'}(s)] \rho_{\alpha\alpha'}^{rs} \\ & + \sum_\beta [V_{\alpha\beta}(r) \rho_{\beta\alpha'}^{rs} - \rho_{\alpha\beta}^{rs} V_{\beta\alpha'}(s)] \\ & + (\varepsilon_\alpha - \varepsilon_{\alpha'}) \rho_{\alpha\alpha'}^{rs} \\ & + i\hbar \left\{ \delta_{\alpha\alpha'} \sum_\mu \sqrt{\Gamma_{\alpha\mu}^{rr}} \rho_{\mu\mu}^{rs} \sqrt{\Gamma_{\alpha\mu}^{ss}} \right. \\ & \left. - \frac{1}{2} \sum_\mu (\Gamma_{\mu\alpha}^{rr} + \Gamma_{\mu\alpha'}^{ss}) \rho_{\alpha\alpha'}^{rs} \right\} \end{aligned}$$

E

$$\begin{aligned} \dot{\rho}_{\bar{\alpha}\bar{\alpha}'}^{rs} = & \delta_{\bar{\alpha}\bar{\alpha}'} \sum_\mu \sqrt{\Gamma_{\bar{\alpha}\mu}^{rr}} \rho_{\mu\mu}^{rs} \sqrt{\Gamma_{\bar{\alpha}\mu}^{ss}} \\ & - \frac{1}{2} \sum_\mu (\Gamma_{\mu\bar{\alpha}}^{rr} + \Gamma_{\mu\bar{\alpha}'}^{ss}) \rho_{\bar{\alpha}\bar{\alpha}'}^{rs} \end{aligned}$$

Expectation value of an observable:  $\langle \hat{\mathcal{O}}(t) \rangle = \text{Tr}[\hat{\mathcal{O}} \hat{\rho}(t)]$

# Coupled-Channels Density-Matrix Approach

## Asymptotic Observables

The probability for producing the target in state  $(I, M_I)$  with the relative coordinate in the direction  $\hat{r}'$ :

$$\begin{aligned} \frac{dW}{d\Omega}(I, M_I) &= \sum_q C_{LmIM_I}^{JM} Y_{Lm}(\hat{r}') \mathcal{S}_{\gamma\lambda}(t_f) \\ &\times C_{L'm'IM_I}^{J'M'} Y_{L'm'}^*(\hat{r}'), \end{aligned}$$

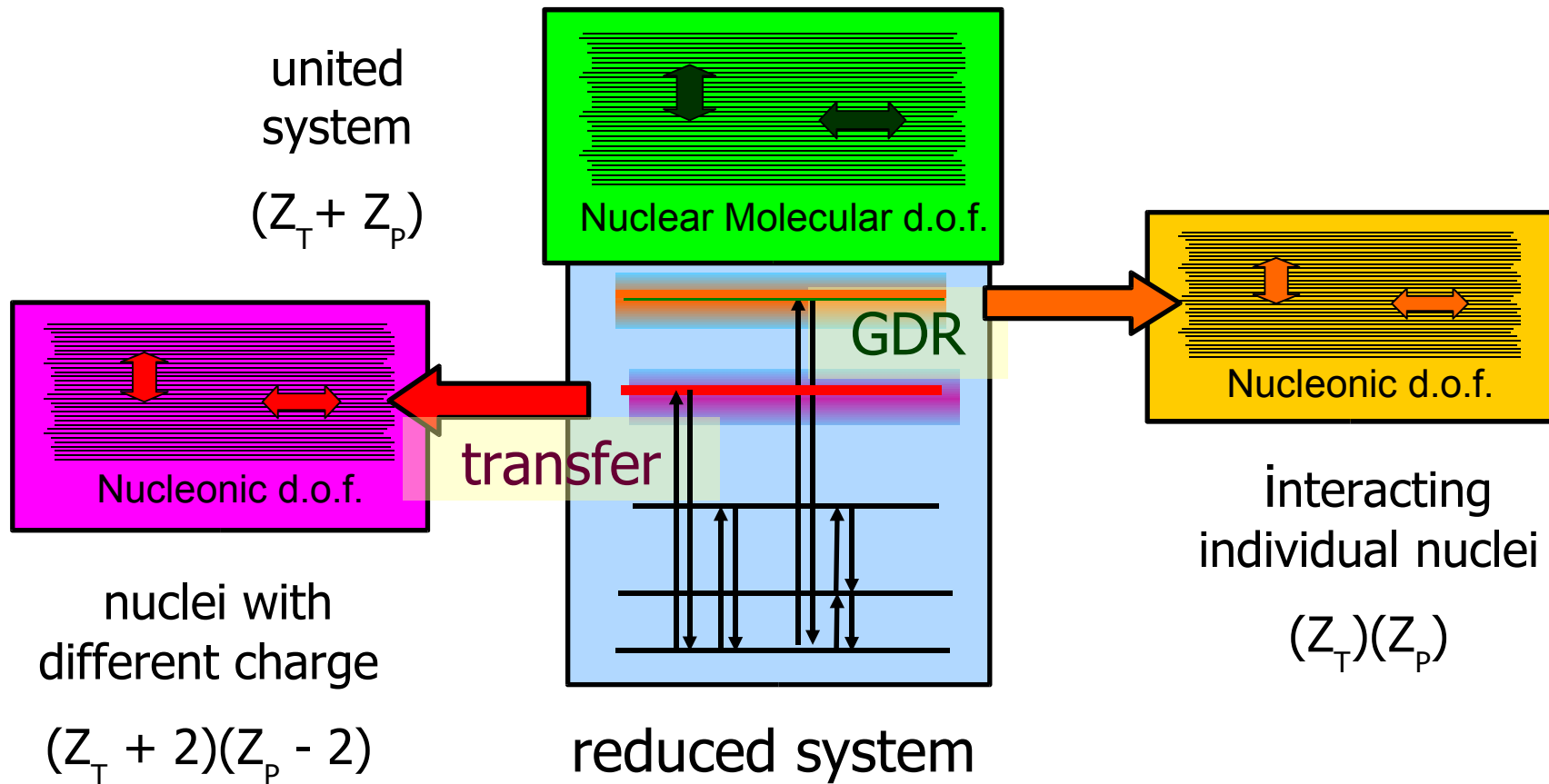
where  $q \equiv (L, m, J, M, L', m', J', M')$ ,  $\gamma \equiv (IL; JM)$ ,  $\lambda \equiv (IL'; J'M')$ , and  $\mathcal{S}_{\gamma\lambda}(t_f) = \sum_{r'} \rho_{\gamma\lambda}^{r'r'}(t_f)$ .

Integrating over all directions  $\hat{r}'$  of solid angles, and summing over all  $M_I$ , the total probability for producing the target in state  $I$  (population) is obtained:

$$W(I) = \sum_{M_I} \sum_{LmJM} (C_{LmIM_I}^{JM})^2 \mathcal{S}_{\gamma\gamma}(t_f)$$

# Coupled-Channels Density-Matrix Approach

## Different Environments

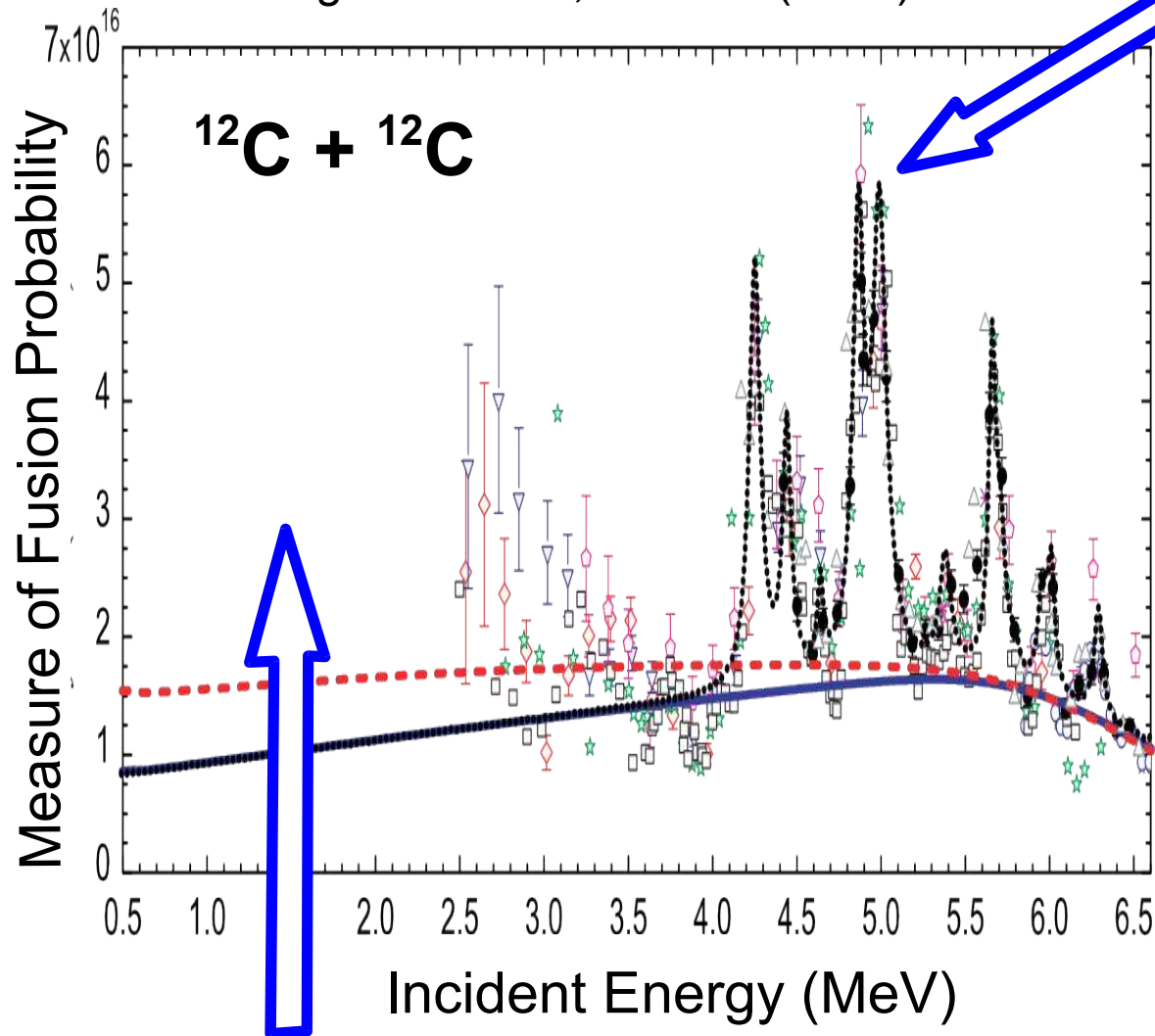


Track decoherence and absorption through different mechanisms  
Environments are specific to particular degrees of freedom

# Application: Understanding fusion of astrophysically-important collisions at low energies

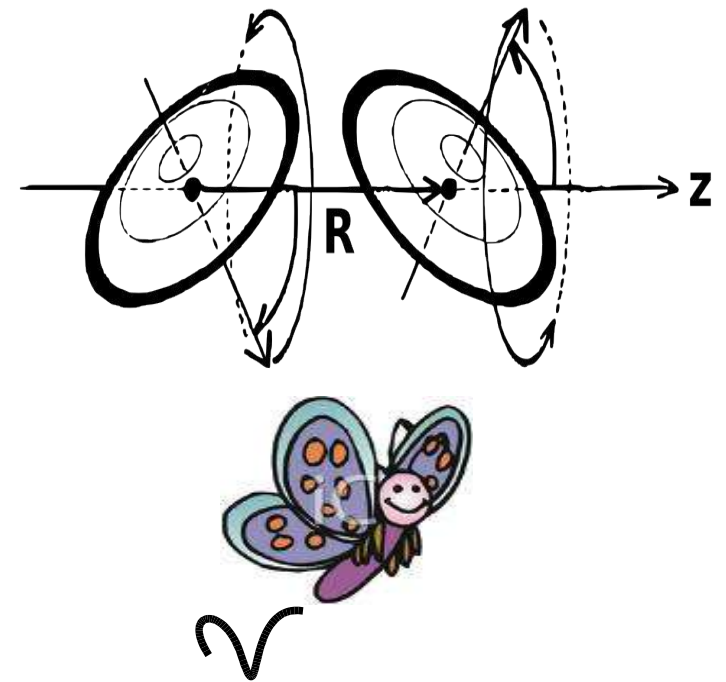
AD-T, Gasques & Wiescher, PLB 652 (2007) 255

E.F. Aguilera et al., PRC 73 (2006) 064601



Origin of the resonances ?

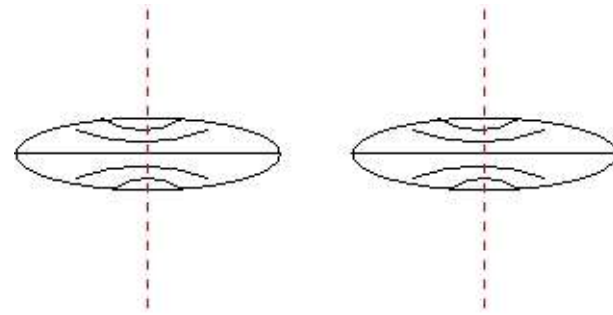
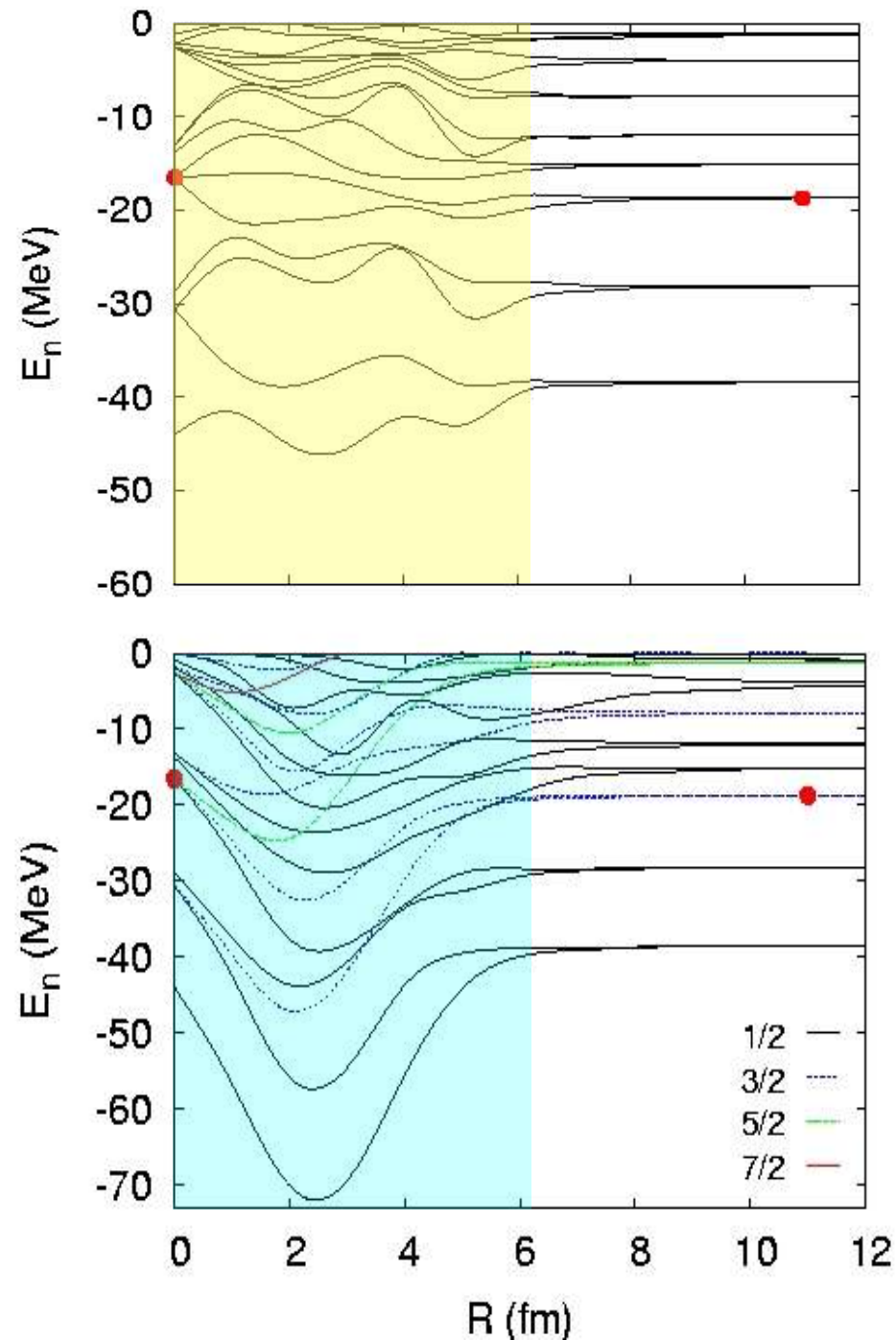
Complex excitation modes  
in dinuclear system



AD-T, PRL 101 (2008) 122501

Fusion probability at astrophysical energies ?

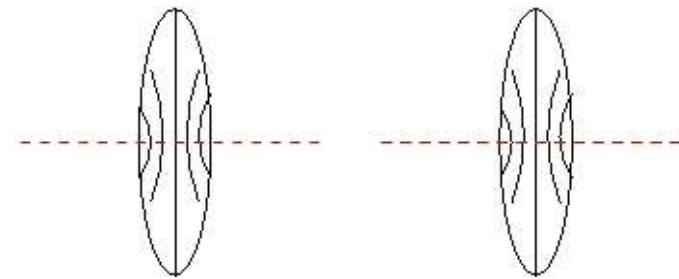
# Neutron molecular shell structure of two interacting deformed $^{12}\text{C}$



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

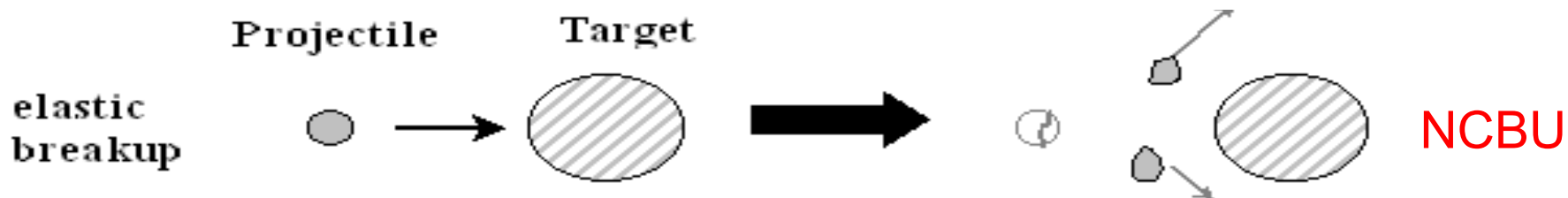
$$V_s \approx \sum_{\nu\mu}^N |s\nu\rangle V_{\nu\mu}^s \langle s\mu|$$

↑





# Application: Unified quantum description of reaction processes of neutron-rich, weakly-bound nuclei



Incomplete fusion



Complete fusion (following breakup)



Complete fusion (without breakup)

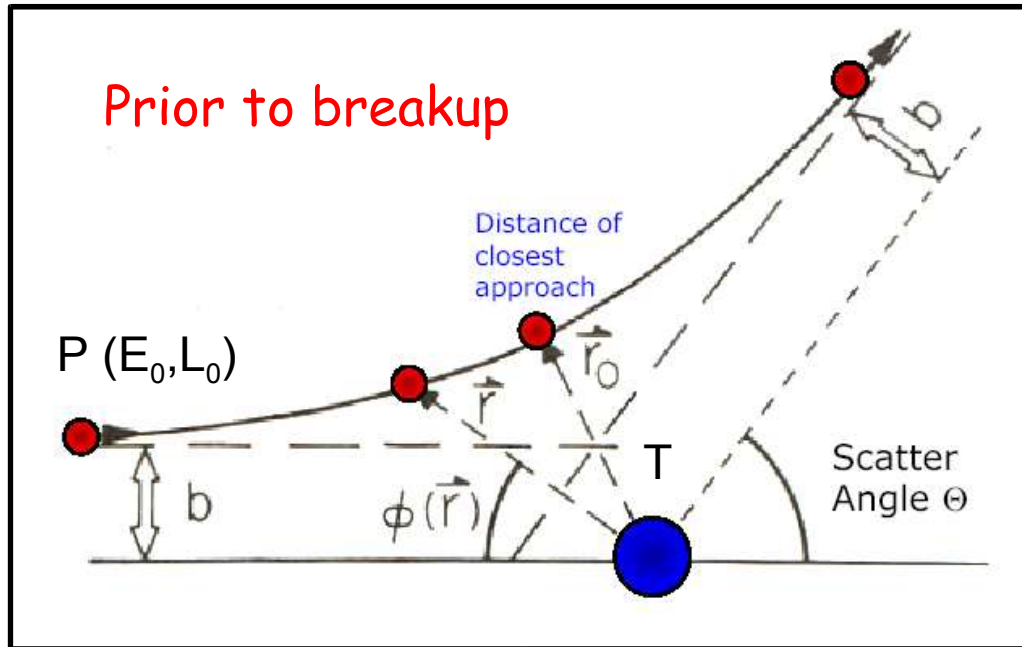


TF

# Classical dynamical model

AD-T, Hinde, Tostevin, Dasgupta & Gasques, PRL 98 (2007) 152701

Quantitative calculations of CF, ICF and NCBU yields above the barrier

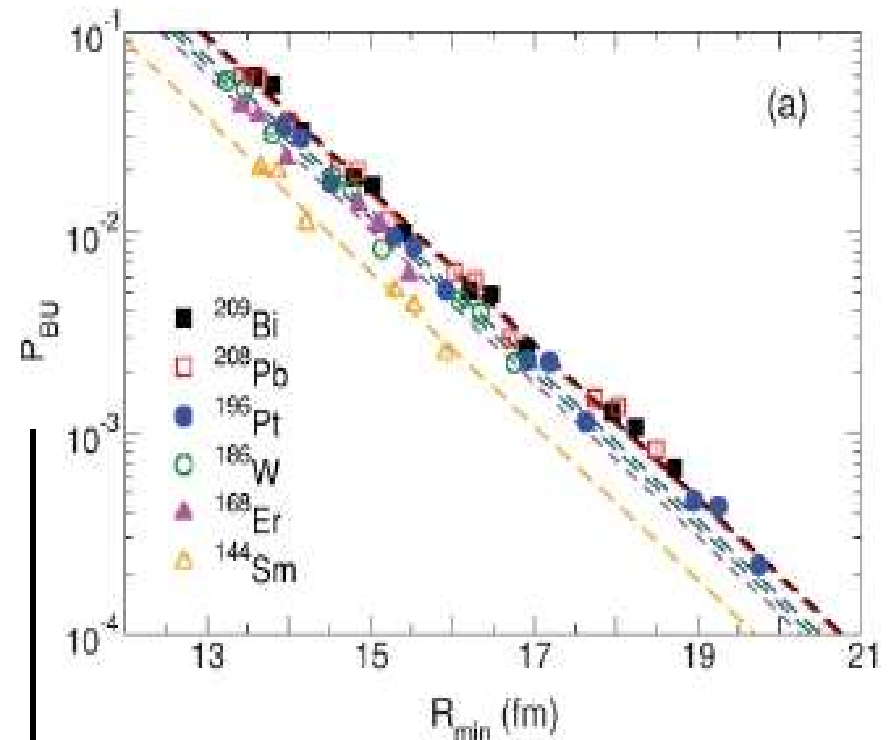


*Main Ingredient :*

$P_{BU}^L(R)dR$  probability of breakup on the interval  $R + dR$

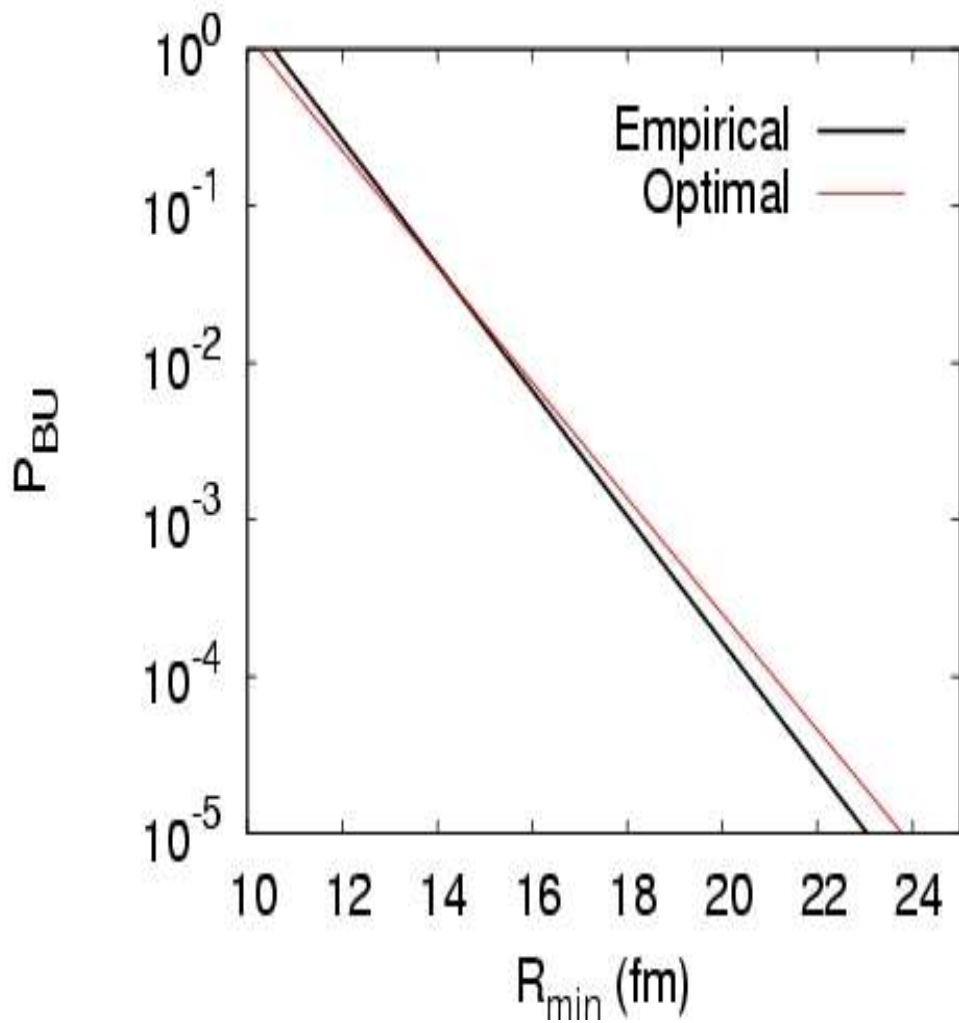
$$P_{BU}(R_{min}) = 2 \int_{R_{min}}^{\infty} P_{BU}^L(R)dR = A \exp(-\alpha R_{min})$$

PHYSICAL REVIEW C 81, 024601 (2010)

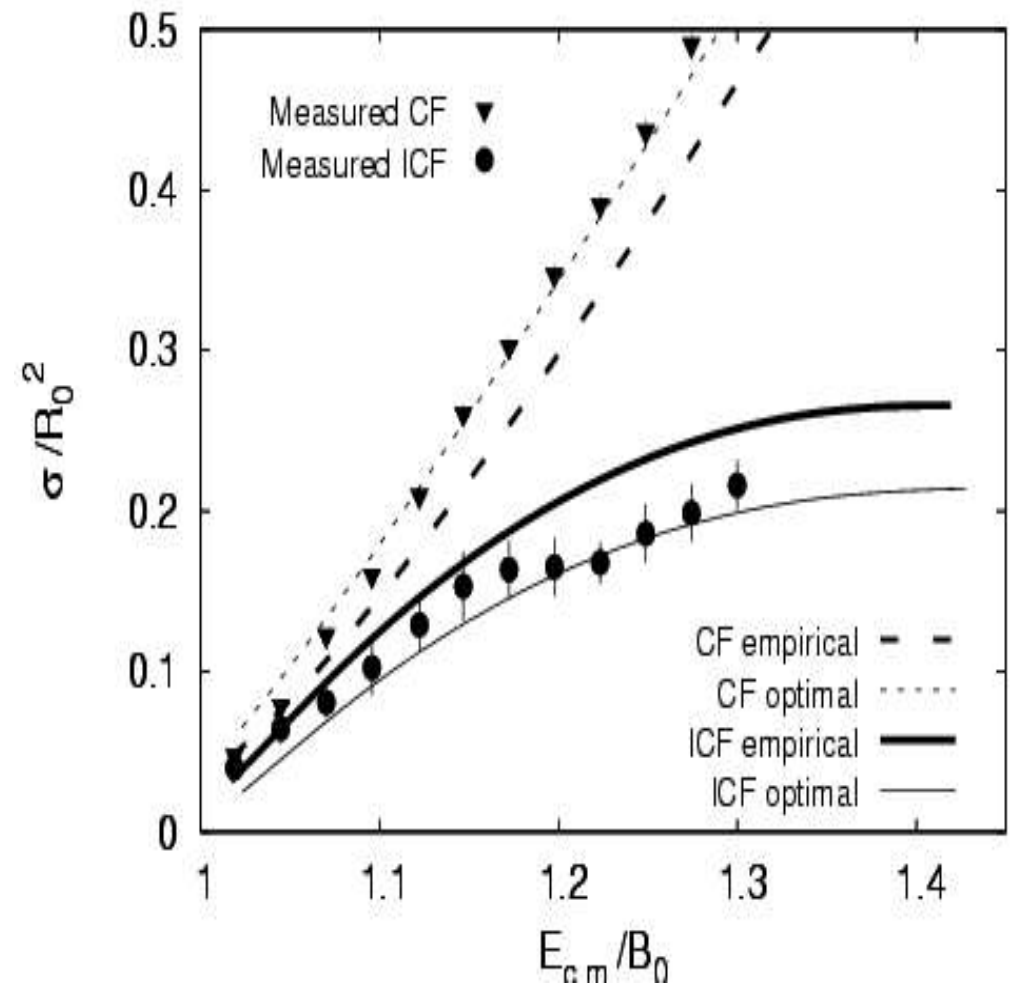


# Fusion excitation functions: “ $^8\text{Be}$ ” + $^{208}\text{Pb}$

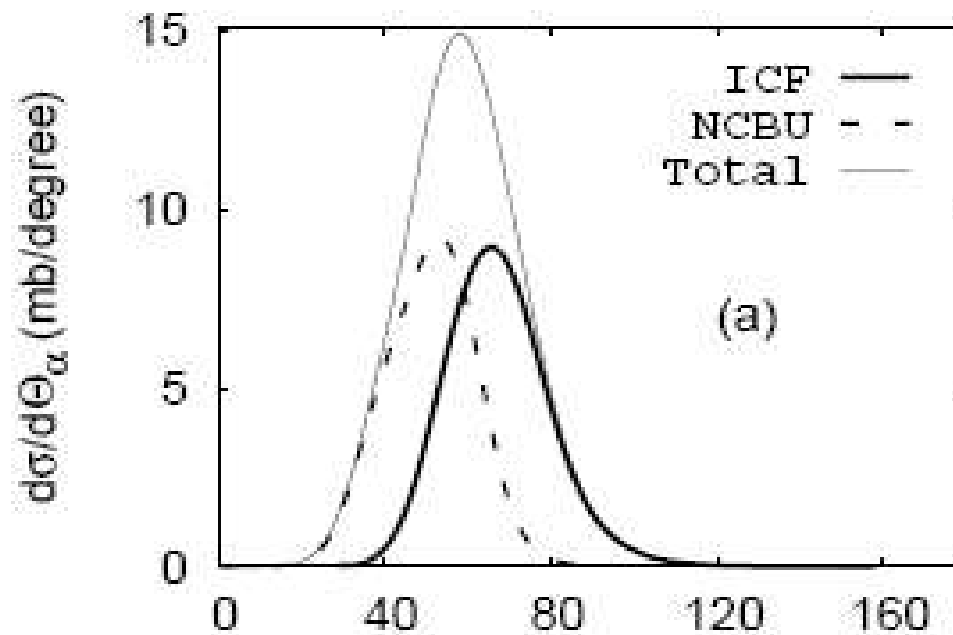
## Breakup function



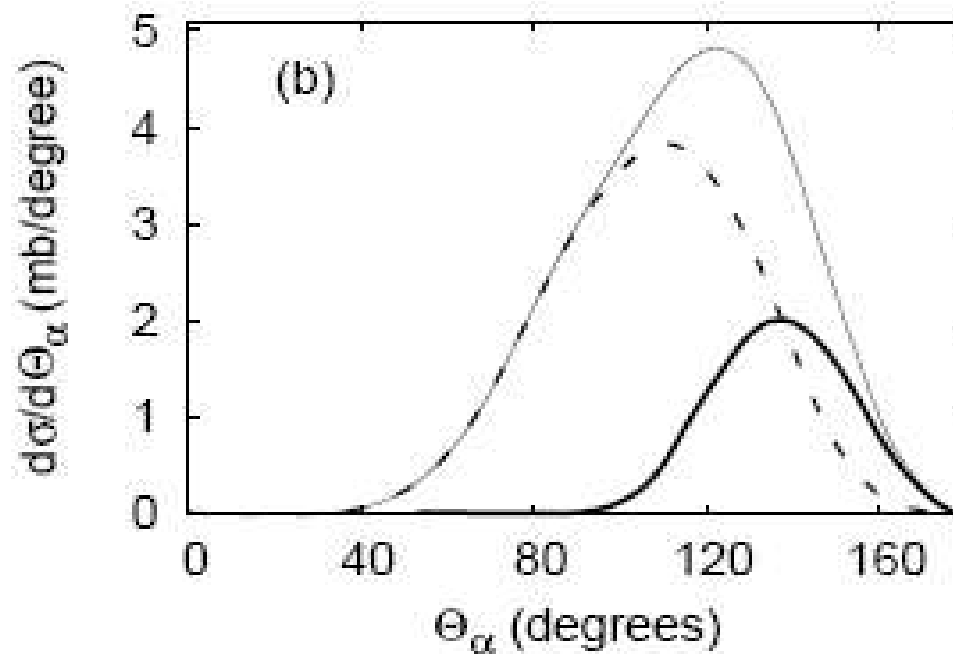
## CF & ICF excitation functions



# Direct alpha-production yields: “ $^8\text{Be}$ ” + $^{208}\text{Pb}$

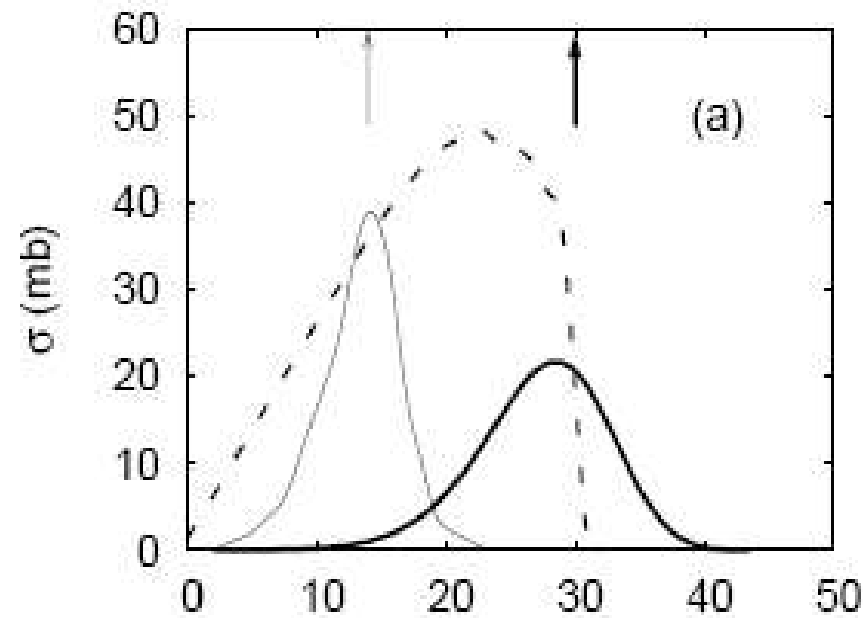


$$E_{\text{cm}}/B_0 = 1.57$$

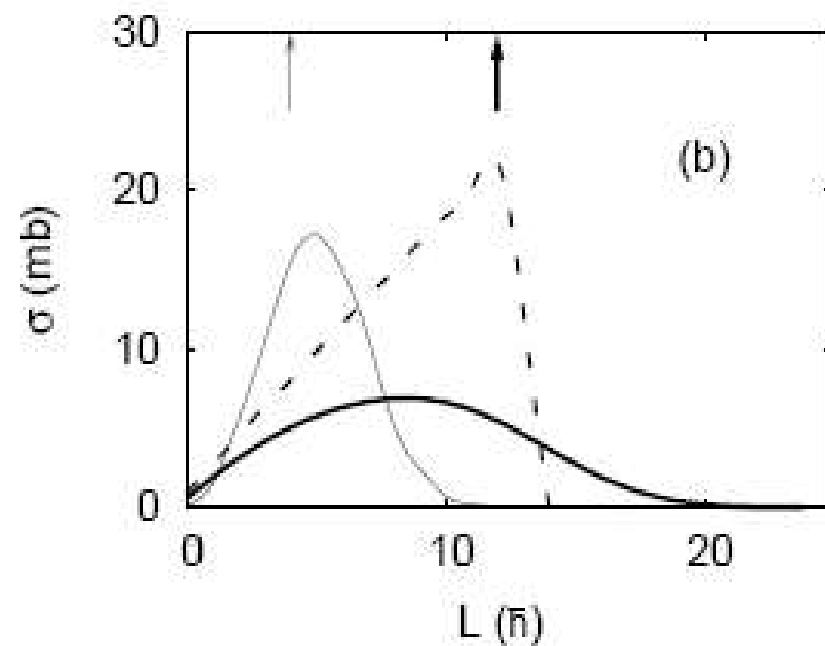


$$E_{\text{cm}}/B_0 = 1.08$$

# Spin distribution of fusion products: $^{216}\text{Rn}$ & $^{212}\text{Po}$

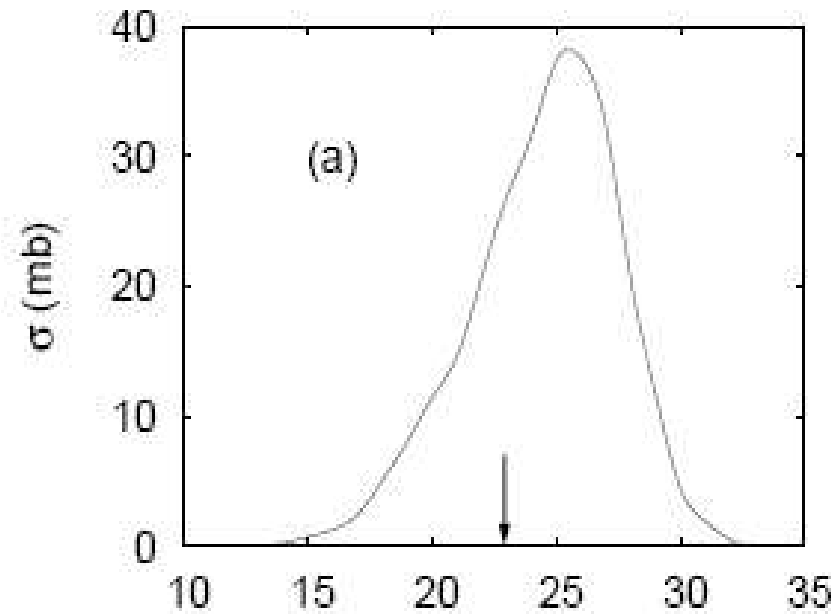


$$E_{\text{cm}}/B_0 = 1.57$$

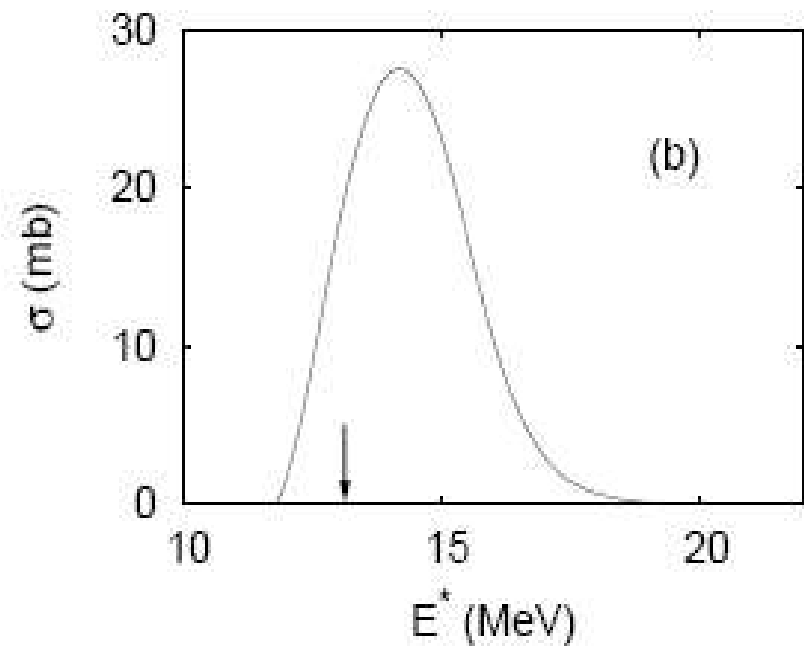


$$E_{\text{cm}}/B_0 = 1.08$$

# Excitation energy distribution of ICF product $^{212}\text{Po}$



$$E_{\text{cm}}/B_0 = 1.57$$



$$E_{\text{cm}}/B_0 = 1.08$$

# Summary

- ★ **Innovative quantum dynamical approach**, which will quantify the **importance of quantum decoherence** in various areas of reaction theory of stable and exotic nuclei
- ★ **Quantum decoherence should always be explicitly included** when modelling low-energy nuclear collision dynamics within a truncated model space of reaction channels
- ★ Links with decoherence in **other quantum systems**

## Workshop on Decoherence in Quantum Dynamical Systems

To be held at ECT\* Trento, IT, April 26<sup>th</sup> – 30<sup>th</sup>, 2010

**Registration: until April 9**

**<http://www.nucleartheory.net/Decoherence/>**

# Breakup probability function

Let us define two probabilities: (i) the probability of breakup between  $R$  and  $R + dR$ ,  $\rho(R)dR$  [being  $\rho(R)$  a density of probability], and (ii) the probability of the weakly-bound projectile's survival from  $\infty$  to  $R$ ,  $S(R)$ . The survival probability at  $R + dR$ ,  $S(R + dR)$ , can be written as follows

$$S(R + dR) = S(R) [1 - \rho(R)dR]. \quad (\text{A.1})$$

Expression (A.1) suggests the following differential equation for the survival probability  $S(R)$ ,

$$\frac{dS(R)}{dR} = -S(R) \rho(R), \quad (\text{A.2})$$

whose solution is [ $S(\infty) = 1$ ]:

$$S(R) = \exp\left(-\int_{\infty}^R \rho(R)dR\right). \quad (\text{A.3})$$

From (A.3), the breakup probability at  $R$ ,  $B(R) = 1 - S(R)$ . If  $\int_{\infty}^R \rho(R)dR \ll 1$ ,  $B(R)$  can be written as

$$B(R) \approx \int_{\infty}^R \rho(R)dR. \quad (\text{A.4})$$

From (A.4), identifying  $\rho(R)$  with  $\mathcal{P}_{BW}^L(R)$ , we obtain expression (1) for the breakup probability integrated along a given classical orbit.



# Measure of Coherence

For a *pure* state described by the state vector  $|\chi\rangle$ :

$$\hat{\rho} = |\chi\rangle\langle\chi|, \text{ and } \text{Tr}(\hat{\rho}) = \langle\chi|\chi\rangle.$$

$$\hat{\rho}^2 = |\chi\rangle\langle\chi|\chi\rangle\langle\chi|, \text{ and } \text{Tr}(\hat{\rho}^2) = \langle\chi|\chi\rangle\langle\chi|\chi\rangle = [\text{Tr}(\hat{\rho})]^2.$$

Hence,  $\text{Tr}(\hat{\rho}^2)/[\text{Tr}(\hat{\rho})]^2 = 1$ , for nonzero values of  $\text{Tr}(\hat{\rho})$ .

For a *mixed* state, there is no single state vector describing the system:

$$\text{Tr}(\hat{\rho}^2)/[\text{Tr}(\hat{\rho})]^2 < 1.$$

The transition from a pure state to a mixed state is caused by decoherence.