Entanglement-Assisted Coherent Control of Bimolecular Scattering

Jiangbin Gong
Department of Chemistry and James Franck Institute
University of Chicago

Paul Brumer
Department of Chemistry and CQIQC
University of Toronto

Four scenarios for controlling collisions

- By tuning the interaction potential with external electric or magnetic fields (e.g.: BEC)
- By laser catalysis (e.g.: H+H2)
- By align/orient reagents (e.g.: Cl+Na2)
- By preparing special initial quantum states

  (**Brumer, Shapiro, Bergmann, Abrashkevish, Gong, Zeman**)

Motivation

- Explore useful quantum effects
- Make connections between QI and QC
- Provide a new ground for testing quantum mechanics in molecular scattering experiments

Entanglement between identical particles:

- Two identical fermions are entangled if their wavefunction cannot be obtained by antisymmetrizing a factorized state.
- Two identical bosons are entangled if their wavefunction is not a product state of the same state and cannot be obtained by symmetrizing a factorized state.

EPR states of two fermions:

	P_s	P_r
S=1: $\uparrow_1 \downarrow_2 + \downarrow_1 \uparrow_2$	+1	-1
S=0: $\uparrow_1 \downarrow_2 - \downarrow_1 \uparrow_2$	-1	+1

spin-dependent cross section with spin-independent Coulomb potential

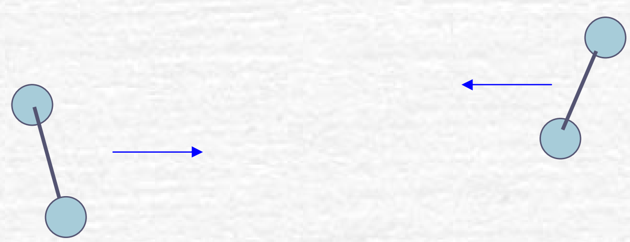
e.g.: proton + proton scattering

proton-proton scattering → molecule-molecule scattering

fermion-fermion scattering → boson-boson scattering

entangled polarization → entangled molecular excitation

para-H2 + para-H2 scattering



para-H2 **para-H2**

Initial entangled state:

$$\frac{1}{\sqrt{2}}\left(|j_1\rangle \otimes |j_2\rangle \pm |j_2\rangle \otimes |j_1\rangle\right) \otimes |m_1 = 0, v_1 = 0\rangle \otimes |m_2 = 0, v_2 = 0\rangle$$

scattering amplitude for entangled initial states

$$f_{\pm}(\hat{\mathbf{R}}) = \frac{1}{\sqrt{2}}\tilde{f}(k'\hat{\mathbf{R}}j_1'm_1'v_1'j_2'm_2'v_2' \leftarrow k\hat{\mathbf{z}}j_1m_1v_1j_2m_2v_2) + \frac{1}{\sqrt{2}}\tilde{f}(k'\hat{\mathbf{R}}j_1'm_1'v_1'j_2'm_2'v_2' \leftarrow k(-\hat{\mathbf{z}})j_2m_2v_2j_1m_1v_1)$$

$$\pm\frac{1}{\sqrt{2}}\tilde{f}(k'\hat{\mathbf{R}}j_1'm_1'v_1'j_2'm_2'v_2' \leftarrow k\hat{\mathbf{z}}j_2m_2v_2j_1m_1v_1) \pm \frac{1}{\sqrt{2}}\tilde{f}(k'\hat{\mathbf{R}}j_1'm_1'v_1'j_2'm_2'v_2' \leftarrow k(-\hat{\mathbf{z}})j_1m_1v_1j_2m_2v_2)$$

$$= \frac{1}{\sqrt{2}}\frac{i\sqrt{\pi}}{\sqrt{kk'}}\sum_{JMm'}\sum_{lj_{12}m_{12}}\sum_{l'j_{12}'m_{12}'}\sqrt{2l+1}\,i^{l-l'}C^{JM}_{l'm'j_{12}'m_{12}'}C^{JM}_{l0j_{12}m_{12}}$$

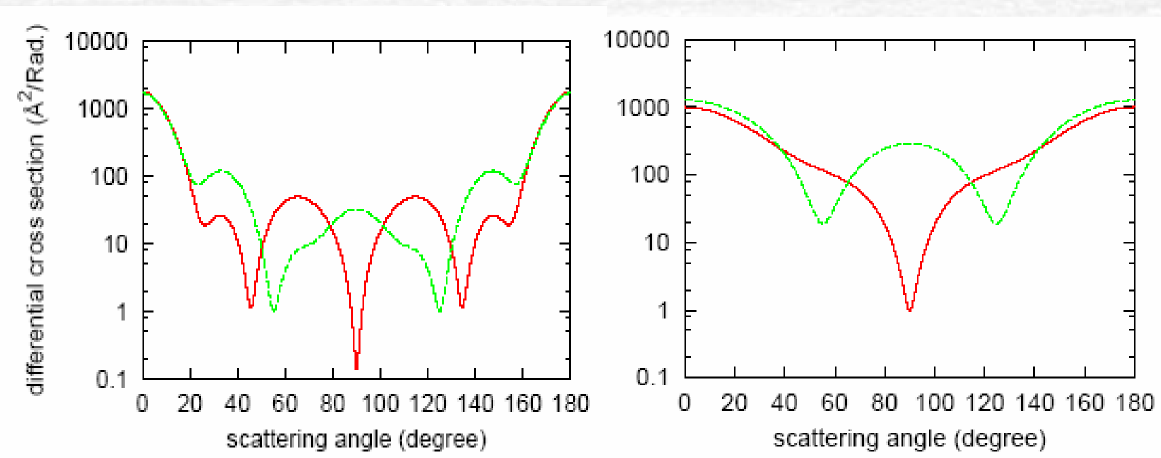
$$\times\{C^{j_{12}m_{12}}_{j_1m_1j_2m_2}[C^{j_{12}'m_{12}'}_{j_1'm_1'j_2'm_2'}Y^{m'}_{l'}(\hat{\mathbf{R}})T^{JM}(j_1'v_1'j_2'v_2'j_{12}'l'|j_1v_1j_2v_2j_{12}l)$$

$$+C^{j_{12}'m_{12}'}_{j_2'm_2'j_1'm_1'}Y^{m'}_{l'}(-\hat{\mathbf{R}})T^{JM}(j_2'v_2'j_1'v_1'j_{12}'l'|j_1v_1j_2v_2j_{12}l)]$$

$$\pm C^{j_{12}m_{12}}_{j_2m_2j_1m_1}[C^{j_{12}'m_{12}'}_{j_1'm_1'j_2'm_2'}Y^{m'}_{l'}(\hat{\mathbf{R}})T^{JM}(j_1'v_1'j_2'v_2'j_{12}'l'|j_2v_2j_1v_1j_{12}l)$$

$$\pm C^{j_{12}'m_{12}'}_{j_2'm_2'j_1'm_1'}Y^{m'}_{l'}(-\hat{\mathbf{R}})T^{JM}(j_2'v_2'j_1'v_1'j_{12}'l'|j_2v_2j_1v_1j_{12}l)]\}.$$

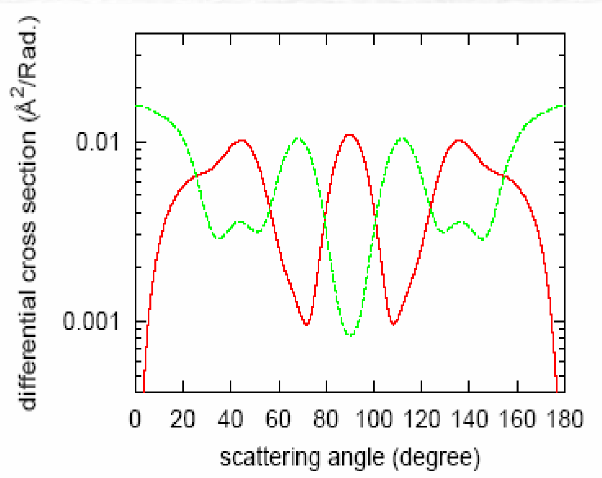
Elastic scattering with entangled initial states



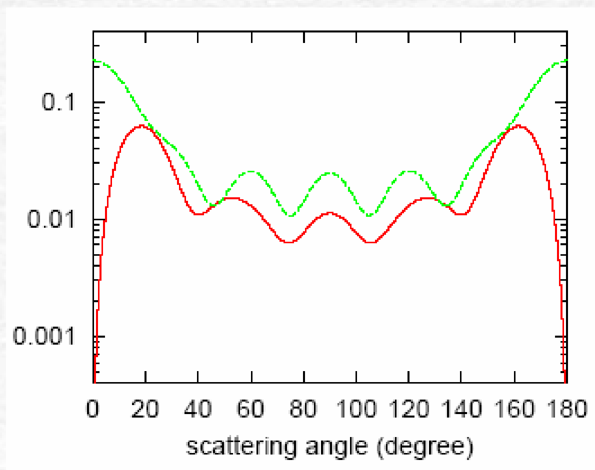
$E = 40\ \mathrm{cm}^{-1}$ $E = 4\ \mathrm{cm}^{-1}$

$j_1 = 0, j_2 = 2$

Inelastic scattering with entangled initial states



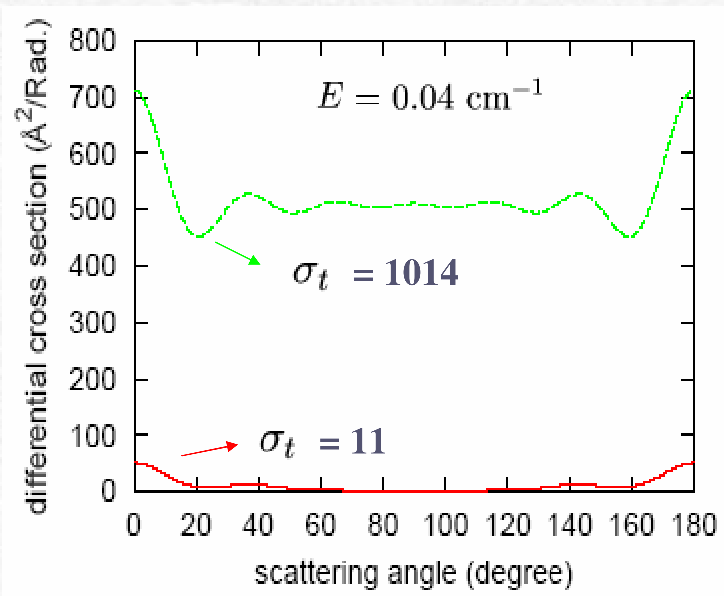
$E = 40 \text{ cm}^{-1}$



$E = 4 \text{ cm}^{-1}$

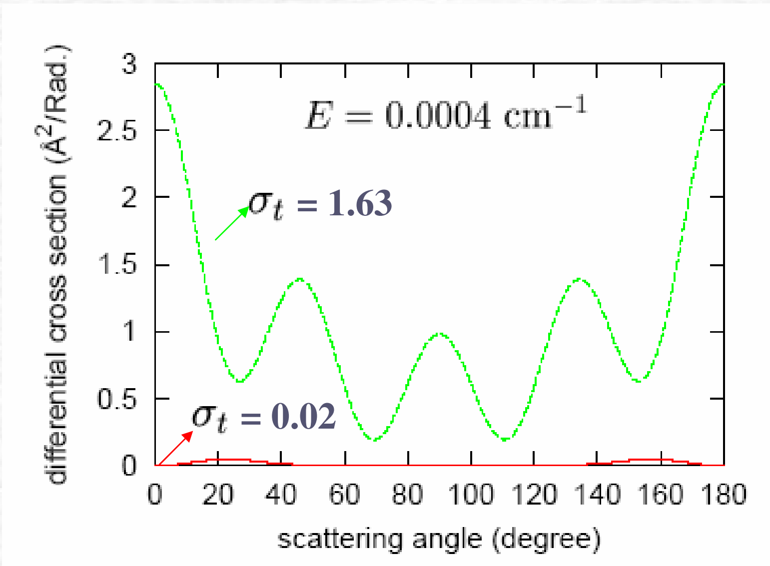
$j_1 = 0, j_2 = 4, j_1' = j_2' = 2$

Ultracold elastic collision



$j_1 = 0, j_2 = 2$

Ultracold inelastic scattering



$j_1 = 0, j_2 = 4, j_1' = j_2' = 2$

A reactive scattering with two channels

F HD

$F + HD \longrightarrow H + FD, \quad D + HF$

Initial entangled state:

$$\frac{1}{\sqrt{2}}\left(|\mathbf{k}_1, \mathbf{K}_1\rangle \otimes |j_1, v_1, m_1\rangle + |\mathbf{k}_2, \mathbf{K}_2\rangle \otimes |j_2, v_2, m_2\rangle\right)$$

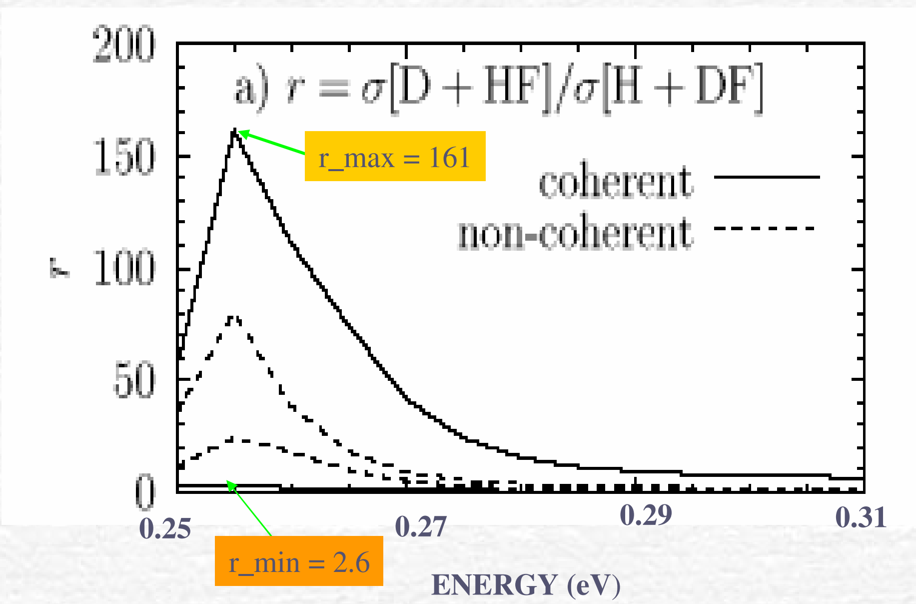
Conditions for interference:

$$\begin{aligned} \frac{\hbar^2 \mathbf{k}_1^2}{2\mu} + e_1(j_1, v_1) &= \frac{\hbar^2 \mathbf{k}_2^2}{2\mu} + e_2(j_2, v_2) \\ \mathbf{K}_1 &= \mathbf{K}_2 \\ m_1 &= m_2 \end{aligned}$$

$$e_1(j_1 = 0, v_1 = 0) = 0.23252 \text{ eV}$$

$$e_2(j_2 = 1, v_2 = 0) = 0.24358 \text{ eV}$$

Entanglement-assisted branching ratio control of reactive scattering



conclusions/comments:

- Collisions often yield undesirable entanglement (decoherence). Here, well-prepared entanglement is used to manipulate collisions.

  In the ultracold limit, even elastic scattering of two para-H2 molecules can be totally shut off.

- To observe entanglement-assisted coherent control of identical particles, one may prepare both scattering particles in appropriate superposition states.

Initial entangled state: $\frac{1}{\sqrt{2}}(|j_1\rangle \otimes |j_2\rangle \pm |j_2\rangle \otimes |j_1\rangle)$

$$\frac{1}{\sqrt{2}}(|j_1\rangle + |j_2\rangle) \otimes \frac{1}{\sqrt{2}}(|j_1\rangle \pm |j_2\rangle) =$$
$$\frac{1}{2}(|j_1\rangle \otimes |j_1\rangle \pm |j_2\rangle \otimes |j_2\rangle) + \frac{1}{2}(|j_1\rangle \otimes |j_2\rangle \pm |j_2\rangle \otimes |j_1\rangle)$$