AtMol
Architecture & Design of Molecule Logic Gates and Atom Circuits
Barcelona (Spain), January 12-13, 2012

Implementing quantum gates and algorithms in ultracold polar molecules

Stéphane Vranckx, P. Pellegrini, L. Bomble, N. Vaeck, M. Desouter-Lecomte

Université Paris Sud 11
Laboratoire de Chimie Physique

Université Libre de Bruxelles
Service de Chimie Quantique et Photophysique

Approach

Aim

— Encoding qubits on electronic, vibrational, rotational and/or hyperfine states of trapped molecules

Approach

Aim

- Encoding qubits on electronic, vibrational, rotational and/or hyperfine states of trapped molecules
- The 2^n states of the n-qubit quantum register are each associated with the population of a specific molecular level
- Logical operations are carried out using laser pulses

Tesch, C. M. et al., *Chemical Physics Letters* **343** (2001)
Bomble, L. et al., *Physical Chemistry Chemical Physics* **18** (2010)

Approach

Aim

- Encoding qubits on electronic, vibrational, rotational and/or hyperfine states of trapped molecules
- The 2^n states of the *n*-qubit quantum register are each associated with the population of a specific molecular level
- Logical operations are carried out using laser pulses

Tesch, C. M. et al., *Chemical Physics Letters* **343** (2001)
Bomble, L. et al., *Physical Chemistry Chemical Physics* **18** (2010)

The number of individually addressable eigenstates necessary increases exponentially with *n*

Approach

Aim

— Encoding qubits on electronic, vibrational, rotational and/or hyperfine states of trapped molecules

— The 2^n states of the *n*-qubit quantum register are each associated with the population of a specific molecular level

— Logical operations are carried out using laser pulses

Tesch, C. M. et al., *Chemical Physics Letters* **343** (2001)
Bomble, L. et al., *Physical Chemistry Chemical Physics* **18** (2010)

The number of individually addressable eigenstates necessary increases exponentially with *n*

Possible solution : network of interacting molecules, each holding a small number of qubits

DeMille, D. *Physical Review Letters* 88 (2002)

Approach

Advantages of polar molecules

— Long range anisotropic dipole-dipole interaction

⇒ Intermolecular communication

— Experimentally : formation, optical trapping and manipulation

Zabawa, P. et al., *Phys. Rev. A* **84** (2011)

Approach

Advantages of polar molecules

— Long range anisotropic dipole-dipole interaction

⇒ Intermolecular communication

— Experimentally : formation, optical trapping and manipulation

Zabawa, P. et al., *Phys. Rev. A* **84** (2011)

Encoding on
NaCs and KRb

Approach

Advantages of polar molecules

— Long range anisotropic dipole-dipole interaction

⇒ Intermolecular communication

— Experimentally : formation, optical trapping and manipulation

Zabawa, P. et al., *Phys. Rev. A* **84** (2011)

⇒ Encoding on NaCs and KRb

Logical operations

— Population transfer using optimized laser pulses

— Determination of the pulses by quantum control techniques

Approach

Advantages of polar molecules

— Long range anisotropic dipole-dipole interaction

⇒ Intermolecular communication

— Experimentally : formation, optical trapping and manipulation

Zabawa, P. et al., *Phys. Rev. A* **84** (2011)

Encoding on
NaCs and KRb

Logical operations

— Population transfer using optimized laser pulses

— Determination of the pulses by quantum control techniques

Using this approach, we implemented intra- and intermolecular quantum gates and algorithms

Encoding

Rovibrational states

— Relatively long lifetime in the fundamental electronic state

Encoding

Rovibrational states

— Relatively long lifetime in the fundamental electronic state

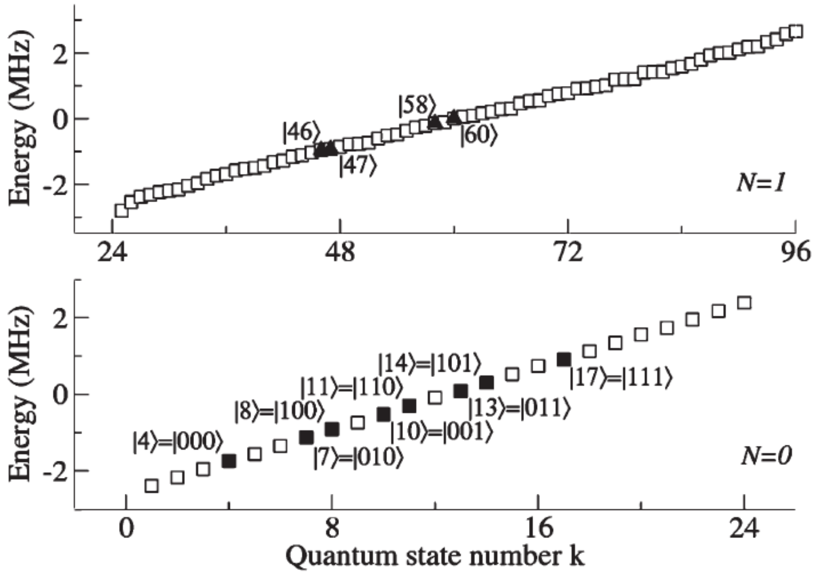
Hyperfine states

— Larger number of states and complex energy structure

— Long lifetime

— Transitions : microwave range

⇒ Better pulse shaping techniques



Pellegrini, P. and Desouter-Lecomte, M. *Eur. Phys. J. D* **64** (2011)

Encoding

Rovibrational states

— Relatively long lifetime in the fundamental electronic state

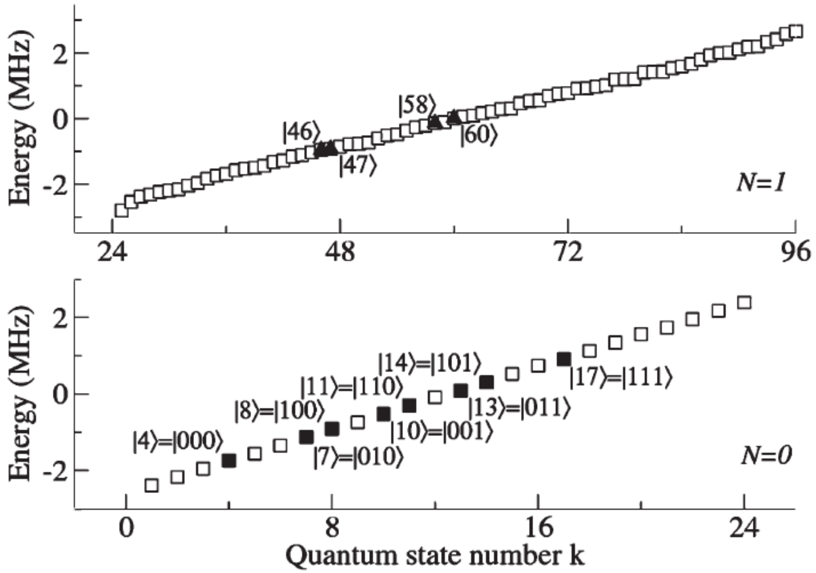
Hyperfine states

— Larger number of states and complex energy structure

— Long lifetime

— Transitions : microwave range

⇒ Better pulse shaping techniques



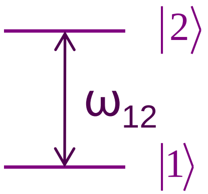
Hyperfine molecular states appear to be promising candidates to encode qubits

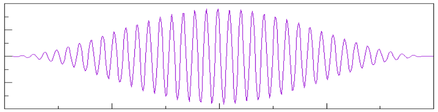
Pellegrini, P. and Desouter-Lecomte, M. *Eur. Phys. J. D* **64** (2011)

Control techniques

π-pulse

- Upon exposition to a (quasi-)resonant laser, a two-level system exhibits Rabbi oscillations
- If the integral of the product of the transition dipole moment and the envelope of the pulse is equal to π : complete population inversion

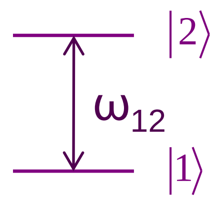


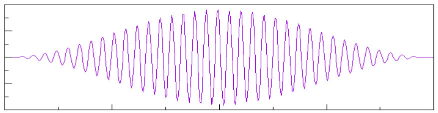


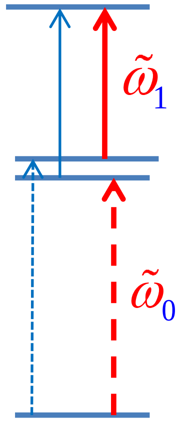
Control techniques

π-pulse

- Upon exposition to a (quasi-)resonant laser, a two-level system exhibits Rabbi oscillations
- If the integral of the product of the transition dipole moment and the envelope of the pulse is equal to π : complete population inversion





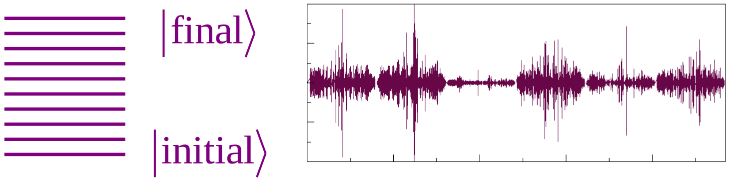


$$\tau_{pulse} > 10 \frac{1}{|\tilde{\omega}_1 - \tilde{\omega}_0|}$$

Control techniques

Multi-Target Optimal Control Theory (OCT)

- Iterative optimization of a functional under constraints
- We simultaneously optimize the performance index for the 2^n input-output transitions as well as a phase constraint
- The laser field is optimized on a time grid
- Constraints on the optimization :
  - The Schrödinger equation must be satisfied at any time
  - Laser field intensity constraint

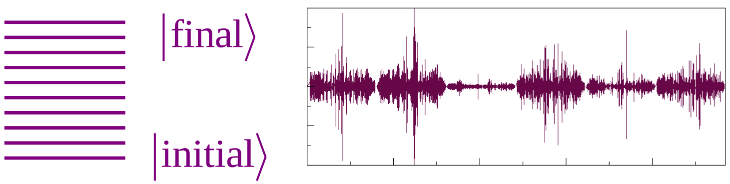


Rabitz, H. Zhu, W., *Journal of Chemical Physics* **109** (1998)

Control techniques

Multi-Target Optimal Control Theory (OCT)

- Iterative optimization of a functional under constraints
- We simultaneously optimize the performance index for the 2^n input-output transitions as well as a phase constraint
- The laser field is optimized on a time grid
- Constraints on the optimization :
  - The Schrödinger equation must be satisfied at any time
  - Laser field intensity constraint



→ Excellent fidelity, but the pulses usually have a complex structure

Model

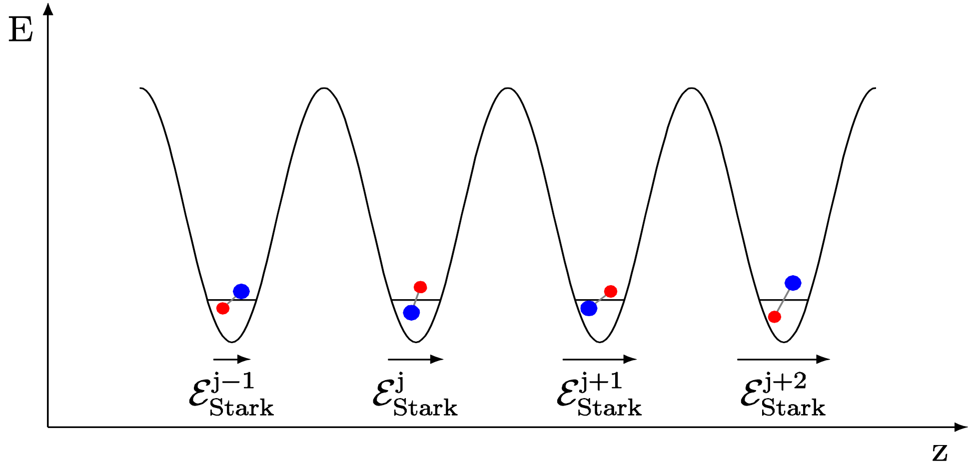
Quantum register

— A string of polar molecules is stored in an optical trap

— An electric field with a gradient along Z differentiates their energy levels and allows individual adressing

— When qubits are encoded on a hyperfine states, a static magnetic field is added to cause their splitting

— In the present calculations, the qubits were encoded on two neighboring molecules



Bomble, L. et al., *Phys. Rev. A* **82** (2010)

Our achievements

On rovibrational levels of NaCs molecules

— Intermolecular 0- and 1-adder using π-pulses

— Intermolecular Deutsch-Josza algorithm using OCT

On hyperfine levels of KRb molecules

— Intramolecular Hadamard and CNOT gates using STIRAP

— Intramolecular Hadamard and CNOT gates using OCT

— Intramolecular 0- and 1-adder using OCT

— Intramolecular 3-qubit version of the Grover algorithm using OCT

— Intermolecular 2-qubit version of the Grover algorithm using OCT

Our achievements

On rovibrational levels of NaCs molecules

- Intermolecular 0- and 1-adder using π-pulses
- Intermolecular Deutsch-Josza algorithm using OCT

On hyperfine levels of KRb molecules

- Intramolecular Hadamard and CNOT gates using STIRAP
- Intramolecular Hadamard and CNOT gates using OCT
- Intramolecular 0- and 1-adder using OCT
- Intramolecular 3-qubit version of the Grover algorithm using OCT
- Intermolecular 2-qubit version of the Grover algorithm using OCT

Bomble, L. et al., *Phys. Rev. A* **82** (2010)

0- and 1-adder

Concept

— Aim : add two binary digits *a* and *b* as well as a carry-in *r* to obtain their sum *s* and a carry-out *r'* for the next iteration

— A full adder requires four qubits, but the problem can be split into a 0-adder and a 1-adder (in that case, whether *b* = 0 or *b* = 1 is determined by the laser pulses)

$r + a + b \longrightarrow s$ and r'

Bomble, L. et al., *Phys. Rev. A* **82** (2010)

0- and 1-adder

Concept

- Aim : add two binary digits *a* and *b* as well as a carry-in *r* to obtain their sum *s* and a carry-out *r'* for the next iteration
- A full adder requires four qubits, but the problem can be split into a 0-adder and a 1-adder (in that case, whether *b* = 0 or *b* = 1 is determined by the laser pulses)

1-adder

Q_1 *r*	Q_2 *a*	Q_3 0	Q_1 *r*	Q_2 *s*	Q_3 *r'*
0	0	0	0	1	0
0	1	0	0	0	1
1	1	0	1	1	1
1	0	0	1	1	0

r +	*a* +	*b* →	*s* and	*r'*
0	0	1	1	0

0- and 1-adder

Concept

— Aim : add two binary digits *a* and *b* as well as a carry-in *r* to obtain their sum *s* and a carry-out *r'* for the next iteration

— A full adder requires four qubits, but the problem can be split into a 0-adder and a 1-adder (in that case, whether *b* = 0 or *b* = 1 is determined by the laser pulses)

1-adder

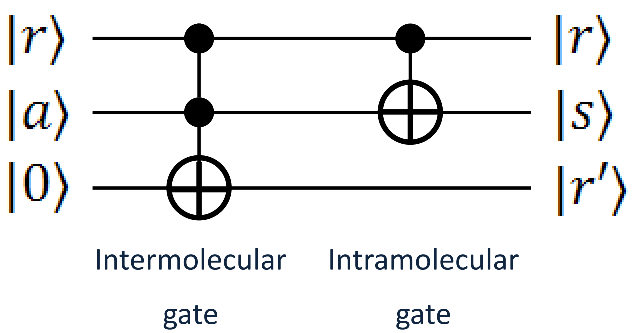
Q_1 *r*	Q_2 *a*	Q_3 0	Q_1 *r*	Q_2 *s*	Q_3 *r'*
0	0	0	0	1	0
0	1	0	0	0	1
1	1	0	1	1	1
1	0	0	1	1	0

r	+	*a*	+	*b*	→	*s*	and *r'*
0		0		1		1	0
1		1		1		1	1

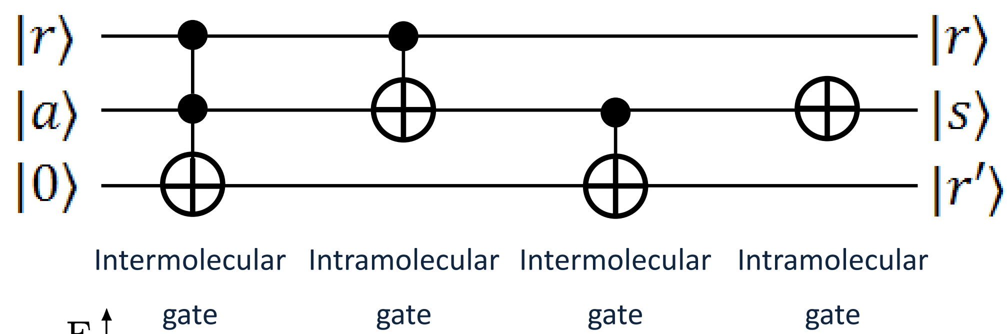
0- and 1-adder

Our implementation

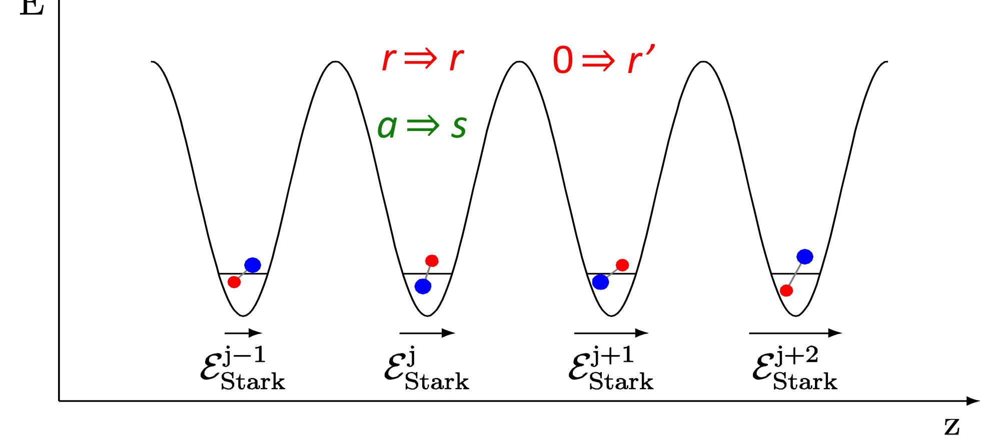
0-adder



1-adder



- Each gate corresponds to a π-pulse
- Encoding :
  - Q_1 : rotation of the molecule j
  - Q_2 : vibration of the molecule j
  - Q_3 : rotation of the molecule j+1

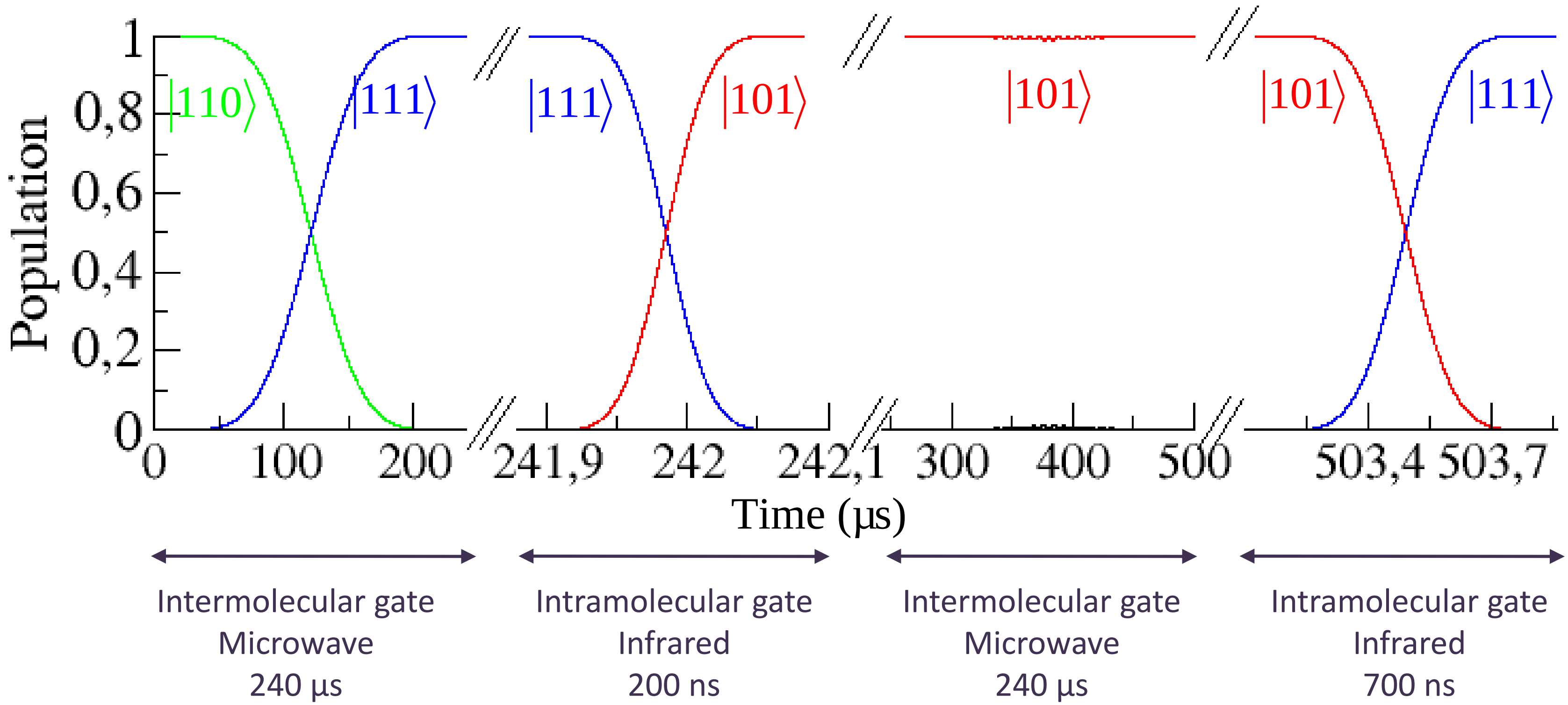


Bomble, L. et al., *Phys. Rev. A* **82** (2010)

0- and 1-adder

Result : 1-adder

$$|r_i\ a_i\ 0\rangle = |1\ 1\ 0\rangle \Rightarrow |r_i\ s_i\ r_{i+1}\rangle = |1\ 1\ 1\rangle$$



Bomble, L. et al., *Phys. Rev. A* **82** (2010)

Our achievements

On rovibrational levels of NaCs molecules

— Intermolecular 0- and 1-adder using π-pulses

— Intermolecular Deutsch-Josza algorithm using OCT

On hyperfine levels of KRb molecules

— Intramolecular Hadamard and CNOT gates using STIRAP

— Intramolecular Hadamard and CNOT gates using OCT

— Intramolecular 0- and 1-adder using OCT

— Intramolecular 3-qubit version of the Grover algorithm using OCT

— Intermolecular 2-qubit version of the Grover algorithm using OCT

Our achievements

On rovibrational levels of NaCs molecules

— Intermolecular 0- and 1-adder using π-pulses

— Intermolecular Deutsch-Josza algorithm using OCT

On hyperfine levels of KRb molecules

— Intramolecular Hadamard and CNOT gates using STIRAP

— Intramolecular Hadamard and CNOT gates using OCT

— Intramolecular 0- and 1-adder using OCT

— Intramolecular 3-qubit version of the Grover algorithm using OCT

— Intermolecular 2-qubit version of the Grover algorithm using OCT

Pellegrini, P.et al., *Phys. Chem. Chem. Phys.* **13** (2011)

Grover's Algorithm

Concept

— Aim : find a specific item S_v among $N=2^n$ elements in an unsorted database

— Each element of the database is associated to a pure state of a *n*-qubit register

— Most efficient classical algorithm : examine each item one by one

⇒ Requires 0,5 *N* tests on average

— Grover's algorithm : quantum parallelization

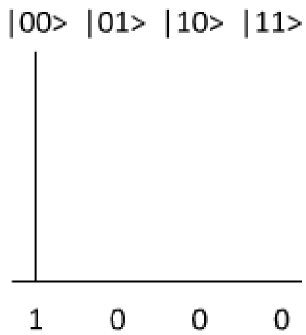
⇒ Requires $O\left(\sqrt{N}\right)$ operations

Pellegrini, P.et al., *Phys. Chem. Chem. Phys.* **13** (2011)

Grover's Algorithm

Our implementation

— We split the algorithm into three steps :



Pellegrini, P.et al., *Phys. Chem. Chem. Phys.* **13** (2011)

Grover's Algorithm

Our implementation

— We split the algorithm into three steps :

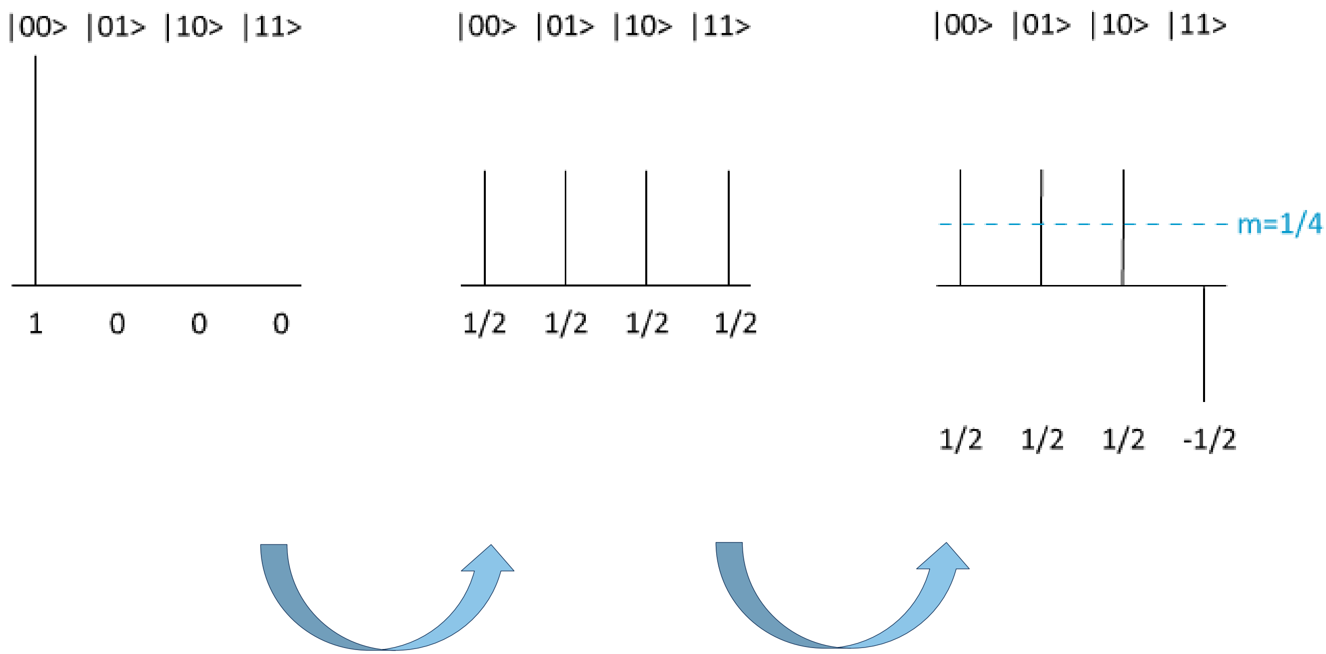
1.Hadamard Gate

Pellegrini, P.et al., *Phys. Chem. Chem. Phys.* **13** (2011)

Grover's Algorithm

Our implementation

— We split the algorithm into three steps :



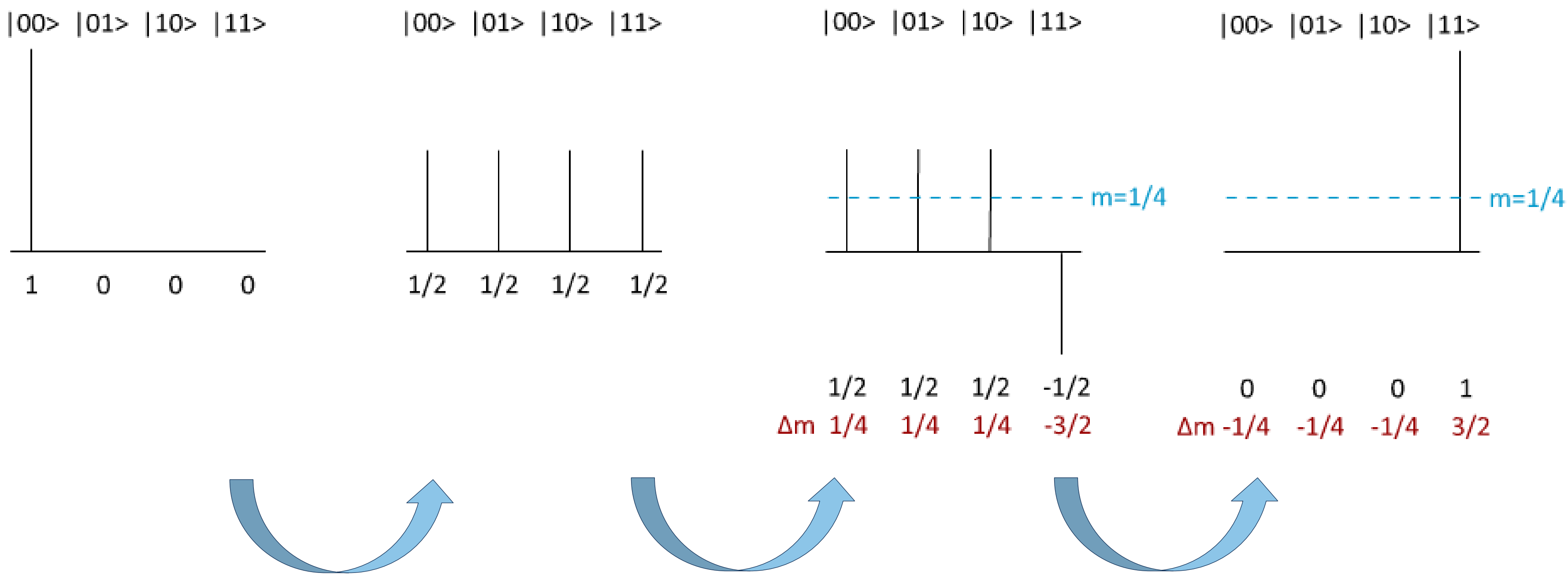
1.Hadamard Gate

2. Phase shift (*Oracle*)

Grover's Algorithm

Our implementation

— We split the algorithm into three steps :

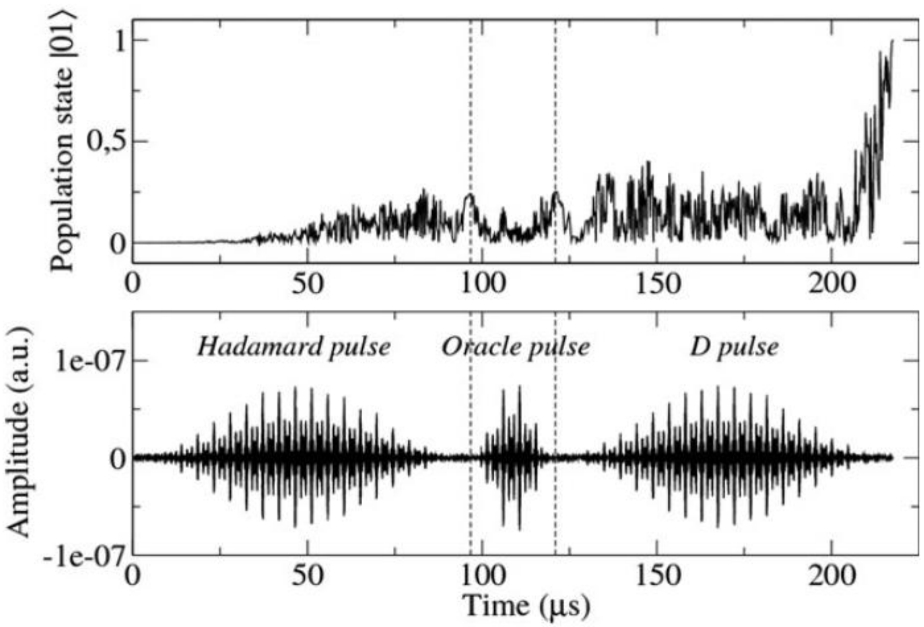


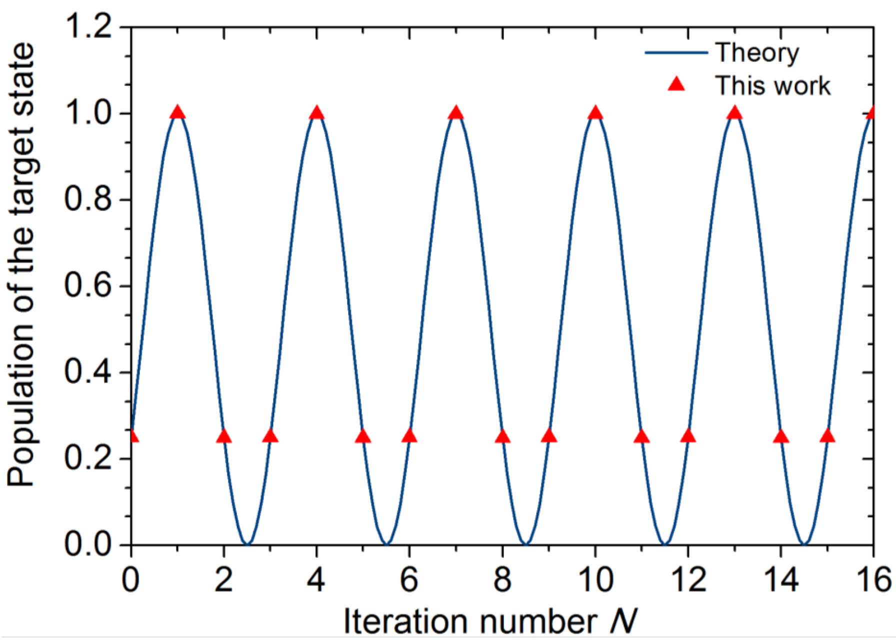
1.Hadamard Gate

2. Phase shift (*Oracle*)

3. Inversion about average (*D pulse*)

Grover's Algorithm





Pellegrini, P.et al., *Phys. Chem. Chem. Phys.* **13** (2011)

Remarks and conclusions

- Using π-Pulses, STIRAP and Optimal Control Theory, we were able to numerically implement both intra- and intermolecular gates and algorithms on rovibrational and hyperfine states of ultracold polar molecules with high fidelity

Remarks and conclusions

— Using π-Pulses, STIRAP and Optimal Control Theory, we were able to numerically implement both intra- and intermolecular gates and algorithms on rovibrational and hyperfine states of ultracold polar molecules with high fidelity

— Encoding qubits on hyperfine states presents several advantages, such as the richness of their energy structure, their long lifetime and the availability of pulse shaping technologies in the microwave regime

Remarks and conclusions

- Using π-Pulses, STIRAP and Optimal Control Theory, we were able to numerically implement both intra- and intermolecular gates and algorithms on rovibrational and hyperfine states of ultracold polar molecules with high fidelity
- Encoding qubits on hyperfine states presents several advantages, such as the richness of their energy structure, their long lifetime and the availability of pulse shaping technologies in the microwave regime
- These results open interesting possibilities toward scalability

Remarks and conclusions

- Using π-Pulses, STIRAP and Optimal Control Theory, we were able to numerically implement both intra- and intermolecular gates and algorithms on rovibrational and hyperfine states of ultracold polar molecules with high fidelity
- Encoding qubits on hyperfine states presents several advantages, such as the richness of their energy structure, their long lifetime and the availability of pulse shaping technologies in the microwave regime
- These results open interesting possibilities toward scalability

Thank you for your attention