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Robust quantum computing using molecules with switchable dipole

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Susanne Yelin, Robin Cote

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Office for Sponsored Programs
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14. ABSTRACT

Of the many systems studied to manipulate quantum information, two ``platforms'' are especially attractive: trapped ions and neutral atoms. Polar molecules represent a new platform that incorporates the best of both and may even bridge the gap with condensed matter physics approaches.

Specific aims: we study the implementation of universal two-qubit logic gates in ultracold polar molecules,

15. SUBJECT TERMS

Ultracold polar molecules, quantum computing, phase gates, dipole switching, coherent control of interactions

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Robin Cote
UU	UU	UU	UU		19b. TELEPHONE NUMBER: 860-486-4912

Report Title

Robust quantum computing using molecules with switchable dipole

ABSTRACT

Of the many systems studied to manipulate quantum information, two ``platforms'' are especially attractive: trapped ions and neutral atoms. Polar molecules represent a new platform that incorporates the best of both and may even bridge the gap with condensed matter physics approaches.

Specific aims: we study the implementation of universal two-qubit logic gates in ultracold polar molecules, focusing on switchable dipole-dipole interactions. With this new system, one may take advantage of the many internal molecular quantum states as qubits to encode and process information.

Findings and Significance: We investigated schemes that exploit the wide range of dipole moments in polar molecules; by selectively exciting transitions from low- to high-dipole states in two molecules, using optical or microwave transitions, the interaction can effectively be controlled. We examined several variations of this scheme in real physical systems, using three examples to highlight the versatility of dipolar molecules in this context. CO, is a system with a small dipole moment in its ground state and a large-dipole excited state. LiH (or molecules with similar properties) has the opposite attributes. Finally, the best scheme might consist of just the lowest lying rotational states of molecules with a large permanent dipole moment. In this case, the ``ground state'' has a truly zero dipole moment. We examined the implementation assuming two potential architectures, optical lattices, and microtraps connected to superconducting wires, in close contact with the groups of Doyle/Lukin (Harvard) and DeMille (Yale). We studied in detail the inverted scheme and the rotational schemes, and examined various sources of error and decoherence, and how they could be controlled or even removed. Finally, we explored how efficient formation of molecules could be controlled: this is important, since one needs ultracold molecules prepared in specific states.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

1- "Analysis of experimental feasibility of polar-molecule-based phase gates",
Elena Kuznetsova, Robin Cote, Kate Kirby, and S. F. Yelin,
Phys. Rev. A 78, 012313 (2008).

2- "Formation of deeply bound molecules via chainwise adiabatic passage",
Elena Kuznetsova, Philippe Pellegrini, Robin Cote, M. D. Lukin, and S. F. Yelin,
Phys. Rev. A 78, 021402(R) (2008).

3- ``Quantum information processing with ultracold polar molecules."
S.F. Yelin, Dave DeMille, and R. Cote,
Book Chapter 17 in Cold Polar Molecules: Creation and Applications, edited by R.V. Krems, W.C. Stwalley, and B. Freidrich, Taylor and Francis (2009).

4- ``Efficient formation of ground state ultracold molecules via STIRAP from the continuum at a Feshbach resonance."
E. Kuznetsova, M. Gacesa, P. Pellegrini, S.F. Yelin, and R. Cote,
New J. Phys. 11, 055028 (2009).

5- ``Phase gate and readout with an atom-molecule hybrid platform."
E. Kuznetsova, M. Gacesa, S. F. Yelin, and R. Cote,
Phys. Rev. A 81, 030301 (2010).

Number of Papers published in peer-reviewed journals: 5.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Number of Papers published in non peer-reviewed journals: 0.00

(c) Presentations

1- R. Cote,
"Quantum Computing with switchable dipoles."
Invited talk, ITAMP-CUA Workshop on Hybrid Approaches to Scalable Quantum Information Systems,
Cambridge (MA), May 24-26, 2007.

2- R. Cote,
"Ultracold polar molecules in a single quantum state."
Invited talk, ITAMP-UBC Workshop on Coherent Control of Ultracold Molecular Processes,
Vancouver (Canada), Wednesday August 1, 2007.

3- R. Cote,
"Evanescent-wave mirrors as controllable traps."
Invited talk, ITAMP Workshop on Quantum Reflection,
Cambridge (MA), October 22-24, 2007.

4- Elena Kuznetsova,
"Polar molecules based phase gates."
Pan American Advanced Studies Institute,
Ultrafast and ultrasmall 2008, Buzios, Brazil,
March 31 to April 11, 2008.

5- Susanne Yelin,
"Quantum information processing and nonlinear optics with
polar molecules."
Invited talk at DAMOP meeting May 2008.

6- Elena Kuznetsova
"Quantum computation schemes based on polar molecules."
DAMOP 2008, Penn State University, May 29-31 2008.
Co-authors: Robin Cote, Kate Kirby, Susanne Yelin.

7- Robin Cote
"Quantum Information using AMO systems."
Invited Tutorial at the Aspen Workshop "Quantum Simulation/Computation with Ultracold Atoms and Molecules",
May 24 to June 14, 2009 (Aspen, CO):
- AMO Tutorial 1: trapped ions (Wednesday June 3 2009).
- AMO Tutorial 2: cold atoms (Wednesday June 3 2009).
- AMO Tutorial 3: cold molecules (Wednesday June 3 2009).

Number of Presentations: 7.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

(d) Manuscripts

Number of Manuscripts: 0.00

Patents Submitted

Patents Awarded

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Elena Kuznetsova	1.00
FTE Equivalent:	**1.00**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Robin Cote	0.08	No
Susanne Yelin	0.08	No
FTE Equivalent:	**0.16**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:.....	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:	0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME PERCENT_SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Final Report

Proposal Number: 50573PHQC
Agreement Number: W911NF0610426
Proposal Title: Robust quantum computing using molecules with switchable dipole
Report Period Dates: 08/30/2006 to 08/31/2009

Principal Investigators: Robin Côté and Susanne Yelin

• Statement of the problem studied

Of the many systems studied to manipulate quantum information, two "platforms" are especially attractive: trapped ions and neutral atoms. Polar molecules present a promising new platform for quantum computation [1, 2, 3, 4, 5], because they incorporate the prime advantages of neutral atoms (scalability to large numbers of bits) and trapped ions (strong interactions), along with the long coherence times characteristic of both. The advances in cooling and storing [6] techniques are beginning to make the precise manipulation of single molecules possible. In addition, polar molecules could be integrated into condensed matter physics architectures, using, for example, molecule-chips or microtraps connected to superconducting wires. In recent articles [3, 4], the experimental implementation of quantum information processing using superconducting stripline resonators has been studied in detail.

The aim of this research project is to perform a detailed investigation of quantum computing schemes based on polar molecules. The long-range dipole-dipole interaction between polar molecules is a crucial ingredient to implement quantum gates. This project focuses on the study of the implementation of universal two-qubit logic gates using switchable dipole-dipole interactions between ultracold polar molecules. With this new system, one may take advantage of the many internal molecular quantum states as qubits to encode and process information.

The problem studied is divided in three main topics: molecular properties required, feasibility of quantum gates under realistic conditions, and finally, the formation/preparation of ultracold polar molecules in the appropriate states. For the first topic, *i.e.* the molecular properties for quantum computing with polar molecules, the general requirements are investigated (*e.g.*, the range of dipole moments required, the selectivity of transitions from low- to high-dipole states in molecules, the use of optical or microwave transitions, etc.). The second topic, *i.e.* feasibility in realistic systems, requires the investigation of molecular systems providing an optimal combination of quantum gate times, coherence times, number of operations, high gate accuracy, and experimental feasibility. Specific molecules are studied for specific excitation schemes in real physical systems, such CO, a system with a small dipole moment in its ground state and a large-dipole excited state, or LiH (or molecules with similar properties), with the opposite attributes. A key point in assessing the feasibility of quantum computing with polar molecules is the analysis of possible sources of error and decoherence, and how they could be controlled or even removed. The third topic, *i.e.* the formation/preparation of ultracold polar molecules, is an important aspect of the project, since one needs ultracold molecules prepared in specific states for quantum information storage and processing. In this last topic, in addition to investigating the means to produce ultracold molecules in targeted states, the coherent manipulation of the molecules between quantum states is also studied, using methods such as STIRAP (stimulated Raman adiabatic passage).

• Summary of the most important results

During the duration of this grant, we have investigated the general properties required for quantum information processing using polar molecules: the results have been published in Physical Review A. Realistic numbers have also been obtained for bi-alkali and alkali-hydride molecules, and a more realistic setting for ground-state only switching has been worked out.

The formation and manipulation of ultracold molecules is a timely and necessary addition to this work. We considered , which a technique called "multistate chainwise stimulated Raman adiabatic passage" as well as STIRAP directly from the continuum using Feshbach Optimized Photoassociation (FOPA). This ensures efficient and robust creation of dense ultracold molecular ensembles in their ground rovibrational state. This work is published as a Phys. Rev. Rapid Communication, and in the New Journal of Physics. We also worked on bridging the gap with condensed matter systems by exploring how polar molecules embedded in solids could be employed: this work is being finalized and written up in a manuscript as well. Finally, we wrote a book chapter on quantum computing with polar molecules.

In details

1. In our first article [P-1] [PRA **78**, 012313 (2008)], we analyzed our proposed physical implementation of a quantum computer based on polar molecules with *switchable* dipoles, *i.e.*, dipole moments that can be switched "on" and "off". We found that conditional dipole-dipole interaction is an efficient tool for realizing two-qubit quantum gates necessary to construct universal gates. We gave a set of general requirements for a molecular system, which would provide an optimal combination of quantum gate times, coherence times, number of operations, high gate accuracy, and experimental feasibility. We proceeded with an analysis of a two-qubit phase gate realization based on switchable dipole-dipole interactions between polar molecules in an optical lattice architecture. We considered one of the schemes proposed in our previous work [5] [PRA **74**, 050301(R) (2006)], using specific molecules, such as CO and NF. We suggested suitable electronic states and transitions, and investigate requirements for the laser pulses driving them. Finally, we analyzed possible sources of decoherence and list practical difficulties of the scheme.

2. In our second article [P-2] [PRA **78**, 021402(R) (2008)], we suggested and analyzed a technique for the efficient and robust creation of dense ultracold molecular ensembles in their ground rovibrational state. In our approach a molecule is brought to the ground state through a series of intermediate vibrational states via a multistate chainwise stimulated Raman adiabatic passage technique. We studied the influence of the intermediate states decay on the transfer process and suggested an approach that minimizes the population of these states, resulting in a maximal transfer efficiency. Numerical analysis suggests a transfer efficiency $> 90\%$, even in the presence of strong collisional relaxation are present in a high density atomic gas.

3. In our third article [P-3] [New J. Phys. **11** 055028 (2009)], we developed a theoretical description of photoassociative stimulated Raman adiabatic passage (STIRAP) near a Feshbach resonance in a thermal atomic gas. In this work based on our previous results on FOPA (Feshbach optimized photoassociation) [7], we showed that it is possible to use low-intensity laser pulses to directly excite pairs of atoms in the continuum near a Feshbach resonance and

to transfer most of the atomic cloud to the lowest rovibrational level of the molecular ground state. For a broad resonance, commonly found in several mixtures of alkali atoms, our model predicts a transfer efficiency up to 97% for a given atom pair, and up to 70% when averaged over an atomic ensemble. The laser intensities and pulse durations needed for such an optimal transfer, $10^2 - 10^3$ W/cm^2 and several microseconds, are easily achievable experimentally. A single pair of STIRAP pulses converts an estimated fraction $f \sim 10^{-6} - 10^{-4}$ of atoms in an atomic ensemble, leading to the production of 10 – 1000 molecules in a large sample of 10^7 atoms. A total of $10^4 - 10^6$ pulse pairs are thus required to transfer most atoms into molecules. Such an efficiency compares with or surpasses currently available techniques for creating stable diatomic molecules, and the versatility of this approach simplifies its potential use for many molecular species.

4. In our fourth article [P-4] [PRA **81**, 030301(R) (2010)], we proposed a combined atom-molecule system, in order to optimize quantum information processing in individual traps such as optical lattices. In particular, gates, initialization, and readout are suggested, using two atoms of different species – one atom carrying the qubit and the other enabling the interaction. We described in some detail the implementation of a two-qubit phase gate in which a pair of atoms is transferred into the ground rovibrational state of a polar molecule with a large dipole moment, thus allowing molecules in adjacent sites to interact via their dipole-dipole interaction. We also discuss how the reverse process could be used as a nondestructive readout tool, an alternative to state-selective ionization. We also expect the combined atomic-molecular system to display a rich many-body behavior due to the presence of three species with independently tunable interactions, including short-range interatomic and long-range dipole-dipole intermolecular ones.

5. In our Book Chapter "Quantum information processing with ultracold polar molecules" [P-5], we give a brief overview of some basic concepts in quantum information processing. We then discuss the application of ultracold polar molecules to the task of constructing quantum information processing devices. We show how to perform universal quantum logic operations, emphasizing the role of the dipole-dipole interaction for implementing two-qubit gates. We also describe limits due to experimental constraints on storage and manipulation of quantum information in such platform.

6. Manuscript (in preparation): "Fast quantum gates with polar molecules embedded in solid-state matrices" by Elena Kuznetsova, Robin Côté, and Susanne Yelin. In this manuscript [P-6], we explore an avenue to increase the strength of the interaction between polar molecules in order to obtain faster phase gates. These two-qubit gates rely on electric dipole-dipole interaction between the polar molecules, and by getting them closer, the interaction strength increases. Much shorter gate times are, therefore, expected for polar molecules doped into solids, such rare-gas matrices, where the spacing between the guest molecules can be several nm, or less. Taking CO and NF molecules as good candidates we arrived at an estimate of several ns for the phase gate time if two molecules are separated by $\sim$ 10 nm. Although with such close spacing the molecules can no longer be addressed individually spatially, we explore the use of spectral addressing with inhomogeneous fields at cryogenic temperatures. This manuscript should be submitted to PRA soon.

• **Publications supported by this grant (labelled as [P- ...]):**

P1. E. Kuznetsova, R. Côté, K. Kirby, and S. Yelin, "Analysis of experimental feasibility of polar molecules-based phase gates." Phys. Rev. A **78**, 012313 (2008).

P2. E. Kuznetsova, P. Pellegrini, R. Côté, M.D. Lukin, and S.F. Yelin, "Formation of deeply bound molecules via chainwise adiabatic passage." Phys. Rev. A 78, 021402(R) (2008).

P3. E. Kuznetsova, M. Gacesa, P. Pellegrini, S.F. Yelin, and R. Côté, "Efficient formation of ground state ultracold molecules via STIRAP from the continuum at a Feshbach resonance." New J. Phys. **11** 055028 (2009).

P4. E. Kuznetsova, M. Gacesa, S. F. Yelin, and R. Côté, "Phase gate and readout with an atom-molecule hybrid platform." Phys. Rev. A **81**, 030301 (2010).

P5. S.F. Yelin, Dave DeMille, and R. Côté, "Quantum information processing with ultracold polar molecules." Book Chapter 17 in *Cold Polar Molecules: Creation and Applications*, edited by R.V. Krems, W.C. Stwalley, and B. Freidrich, Taylor and Francis (2009).

P6. E. Kuznetsova, R. Côté, and S. Yelin, "Fast quantum gates with polar molecules embedded in solid-state matrices." In preparation: to be submitted in Phys. Rev. A.

Finally, in addition to the publication mentioned above, the work funded by this grant was presented at several conferences and workshops. We list below the talks and posters presented. Some of the results were also presented at several other invited talks at various institutions, but we do not list them here.

• **Invited talks at meetings**

- R. Côté "Quantum Information using AMO systems." Invited Tutorial at the Aspen Workshop *Quantum Simulation/Computation with Ultracold Atoms and Molecules*, May 24 to June 14, 2009 (Aspen, CO):
  - AMO Tutorial 1: trapped ions (Wednesday June 3 2009).
  - AMO Tutorial 2: cold atoms (Wednesday June 3 2009).
  - AMO Tutorial 3: cold molecules (Wednesday June 3 2009).
- E. Kuznetsova "Quantum computation schemes based on polar molecules." DAMOP 2008, Penn State University, May 29 – 31 (2008).
- S. Yelin, "Quantum information processing and nonlinear optics with polar molecules." Invited talk at DAMOP meeting May 2008.
- E. Kuznetsova "Polar molecules based phase gates." Pan American Advanced Studies Institute, Ultrafast and ultrasmall 2008, Buzios, Brazil, March 31 – April 11, 2008.
- R. Côté "Evanescent-wave mirrors as controllable traps." Invited talk, ITAMP Workshop on *Quantum Reflection*, Cambridge (MA), October 22-24, 2007

- R. Côté "Ultracold polar molecules in a single quantum state." Invited talk, ITAMP-UBC Workshop on *Coherent Control of Ultracold Molecular Processes*, Vancouver (Canada), Wednesday August 1, 2007.

- R. Côté "Quantum Computing with switchable dipoles." Invited talk, ITAMP-CUA Workshop on *Hybrid Approaches to Scalable Quantum Information Systems*, Cambridge (MA), May 24-26, 2007

- **Conferences/Posters**

  - Elena Kuznetsova, Marko Gacesa, Susanne Yelin, and Robin Côté, "Phase gate and readout with an atom/molecule hybrid platform." Session R3: Focus Session: Hybrid and Condensed Matter Quantum Systems (10:30 AM12:30 PM, Friday, May 28, 2010). Contributed talk (E. Kuznetsova) R3.00006, 12:06 PM12:18 PM, DAMOP 2010, May 25-29 2010, Houston (Texas).

  - Elena Kuznetsova, Susanne F. Yelin, and Robin Côté, "Robust quantum computing using molecules with switchable dipoles." Poster Session (Tuesday August 18), ARO Contractor's meeting, Minneapolis August 17-21 2009.

  - Elena Kuznetsova, Marco Gacesa, Philippe Pellegrini, Robin Côté, Mikhail D. Lukin, and Susanne F. Yelin, "Coherent formation of ultracold molecules in the ground rovibrational state." Session E1: Poster Session I (4:00 - 6:00 pm), Poster E1.00050, Wednesday, May 20 2009, DAMOP 2009, May 1923 2009, Charlottesville (Virginia).

  - Elena Kuznetsova, P. Pellegrini, R. Côté, M D. Lukin, and S.F. Yelin, "Formation of deeply bound molecules via chainwise adiabatic passage." ICAP 2008 poster TH82, Poster Session III (Tuesday, July 31), Book of Abtract p.407, Storrs (July 27-August 1 2008).

  - Elena Kuznetsova, R. Côté, Kate Kirby, and S.F. Yelin, "Quantum phase gates with polar molecules in an optical lattice." ICAP 2008 poster MO92, Poster Session I (Monday, July 28), Book of Abtract p.145, Storrs (July 27-August 1 2008).

  - E. Kuznetsova, R. Côté, K. Kirby, and S. Yelin "Quantum computation schemes based on polar molecules." Session C6: Quantum Computation, Contributed talk (E. Kuznetsova) C6.00006, 2:00 PM – 4:24 PM, Wednesday, May 28, 2008, DAMOP 2008 (Penn. State).

References

[1] D. DeMille, *Quantum Computation with Trapped Polar Molecules,* Phys. Rev. Lett. **88**, 067901 (2002).

[2] C. Lee and E. A. Ostrovskaya, *Quantum computation with diatomic bits in optical lattices,* Phys. Rev. A **72**, 062321 (2005).

[3] A. André, D. DeMille, J. M. Doyle, M. D. Lukin, S. E. Maxwell, P. Rabl, R. J. Schoelkopf, and P. Zoller, *A coherent all-electrical interface between polar molecules and mesoscopic superconducting resonators,* Nature Phys. **2**, 636 (2006).

[4] R. Côté, *Quantum information processing - Bridge between two lengthscales*, News & Views, Nature Phys. **2**, 583 (2006).

[5] S.F. Yelin, K. Kirby, and R. Côté, *Schemes for robust quantum computation with polar molecules*, Phys. Rev. A **74**, 050301(R) (2006).

[6] D. DeMille, D.R. Glenn, and J. Petricka, *Microwave traps for cold polar molecules,* Eur. Phys. J. D **31**, 375-384 (2004).

[7] Philippe Pellegrini,, Marko Gacesa, and R. Côté, *Giant formation rates of ultracold molecules via Feshbach Optimized Photoassociation*, Phys. Rev. Lett. **101**, 053201 (2008).