## Implementing quantum gates and algorithms in ultracold polar molecules

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Increasing the number of qubits encoded on a single molecule is challenging as this requires an exponential rise of the number of individually addressable eigenstates. A way to circumvent this problem and to ensure scalability would be to use a network of molecules, each carrying a limited number of qubits and interacting selectively through intermolecular gates. Polar molecules are promising systems for this approach [1] thanks to their strong anisotropic dipole moment and to recent experimental progresses which allow for their preparation in a single state and their manipulation with unprecedented accuracy [2].

We numerically investigate the possibility of implementing quantum algorithms in registers of ultracold polar molecules trapped in an optical lattice with laser pulses (fig. 1). The qubits are encoded either in rovibrational states or in hyperfine states in a static magnetic field by modulating the eigenenergies by a strong Stark field with a gradient to distinguish each molecule. The dipolar interaction induces entanglement between neighboring pendular states. In a first example, the qubits are encoded in states of two neighbouring NaCs molecules [3]. We implement quantum arithmetic gates, a 0– and a 1–adder by using  $\pi$  pulses as well as the Deutsch-Josza algorithm by pulses built by Optimal Control Theory (OCT).

In a second example, we investigate the implementation of logical gates in hyperfine states in the first two rotational manifolds of the ground vibrational level of <sup>85</sup>Rb<sup>133</sup>Cs, <sup>40</sup>K<sup>87</sup>Rb and <sup>41</sup>K<sup>87</sup>Rb molecules exposed to a magnetic field using either STIRAP or Optimal Control Theory [4,5] and by running quantum arithmetic algorithms in hyperfine states of <sup>41</sup>K<sup>85</sup>Rb and <sup>41</sup>K<sup>87</sup>Rb using OCT [6]. Finally, we implement an intermolecular version of the 2-qubit Grover search algorithm in hyperfine states of two neighbouring <sup>41</sup>K<sup>87</sup>Rb molecules trapped in an optical lattice [6]. Our simulations show that high fidelity logic gates can be operated on a timescale of a few tens of microseconds at most. Moreover, all transitions occur in the microwave domain, in which pulse shaping technologies are available.

## References

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## Figures

Fig. 1 - Schematic of a polar molecule based

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