Quantum simulators with ultracold polar molecules and Rydberg atoms

Michał Tomza

Faculty of Physics, University of Warsaw

25th European Conference on Few-Body Problems in Physics
Mainz, August 1, 2023

Why ultracold?

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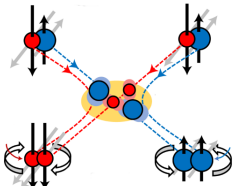
Controlled chemical reactions



Nature Chem. 13, 435 (2021)

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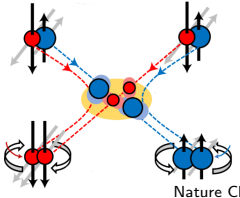

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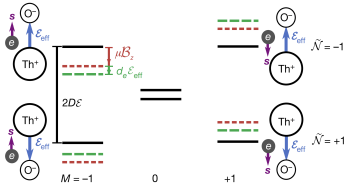
Precision measurements



Nature 562, 355 (2018)

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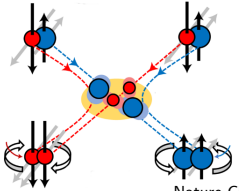

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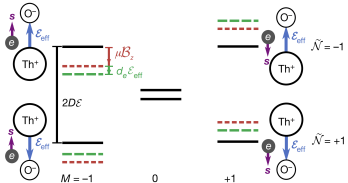

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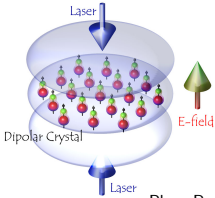
Quantum many-body physics



Phys. Rev. A 76, 043604 (2007)

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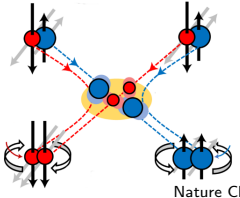

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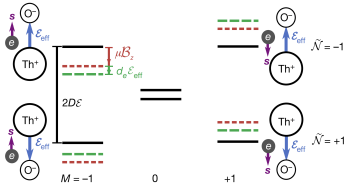

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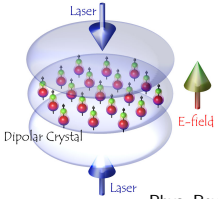

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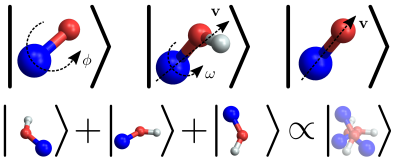
Quantum computing



Phys. Rev. X 10, 031050 (2020)

Theory of ultracold atoms, ions, and molecules

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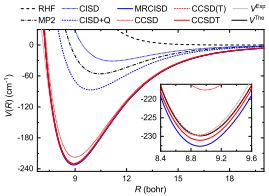
Accurate ab initio calculations



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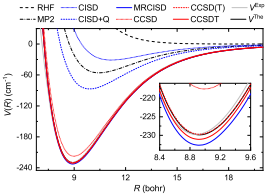
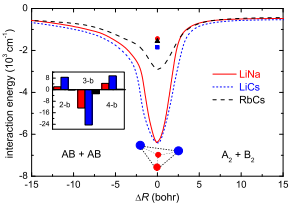


Collisions and chemical reactions



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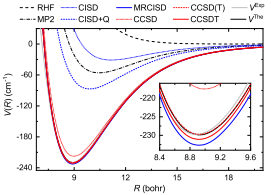

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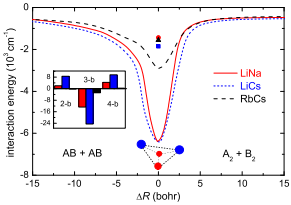
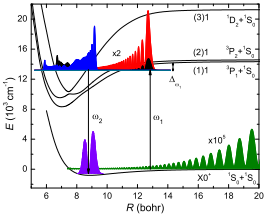


Formation and control of molecules



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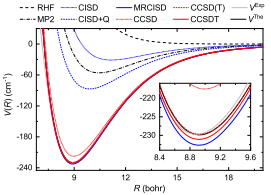

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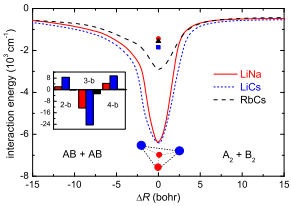

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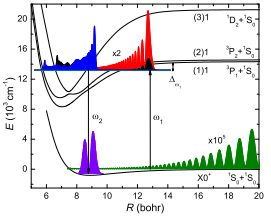
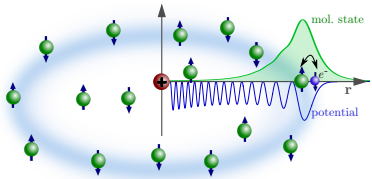


Few-body quantum dynamics



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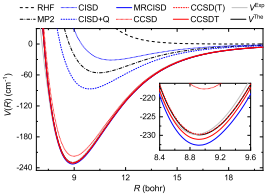

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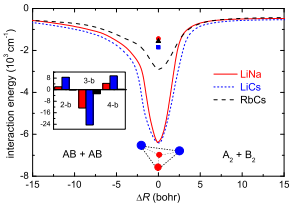

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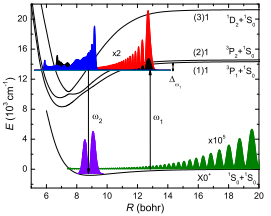

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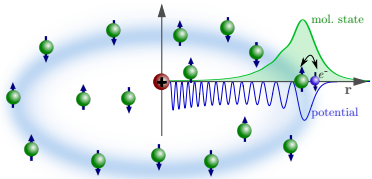
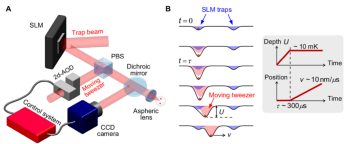
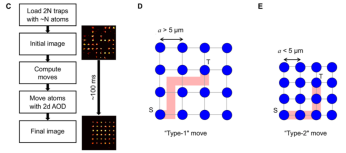


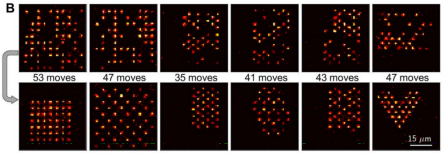
Atoms and molecules
in **optical tweezers**

Atom-by-atom and molecule-by-molecule assembled defect-free arrays

Science 354, 1021 (2016) / Science 354, 1024 (2016)







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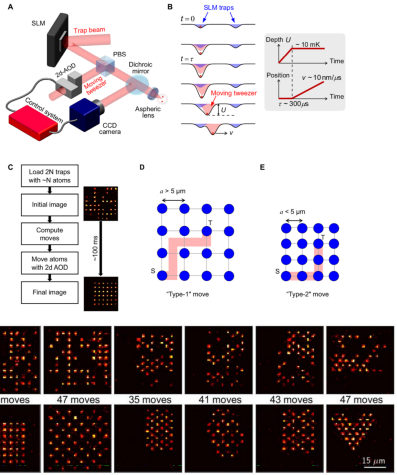
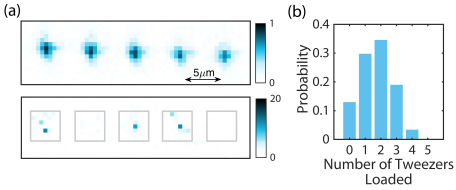


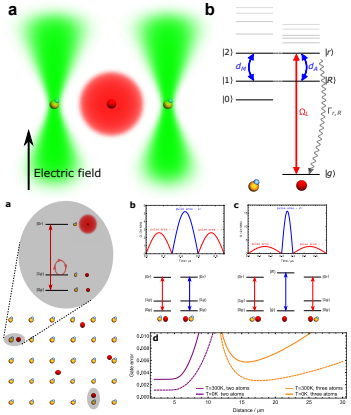
Science 360, 900 (2018) / Science 365, 1156 (2019)



Mixing Rydberg atoms **and** ground-state molecules

Recent theory proposals – Rydberg as a mediator for quantum comp.

C. Zhang, M.R. Tarbutt, PRX Quantum 3, 030340 (2022)



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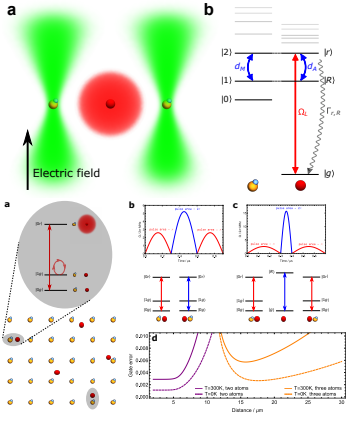
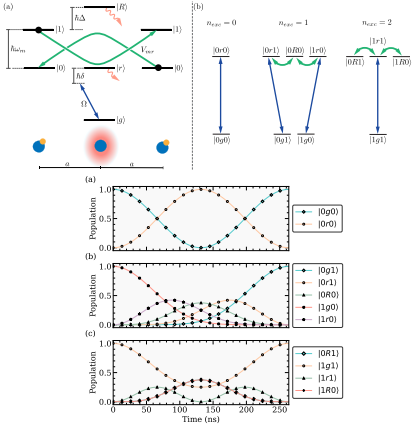


K. Wang, C. P. Williams, L. R.B. Picard, N. Y. Yao, K.-K. Ni, PRX Quantum 3, 030339 (2022)



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Very recent Rydberg-molecule interaction observation!

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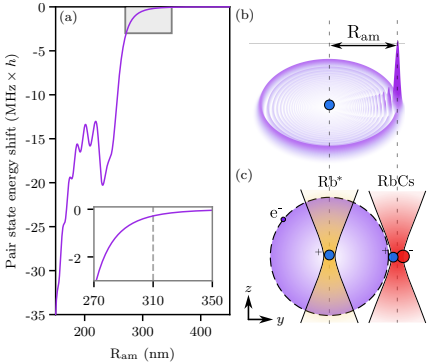

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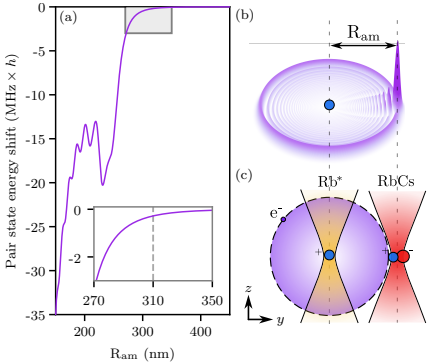
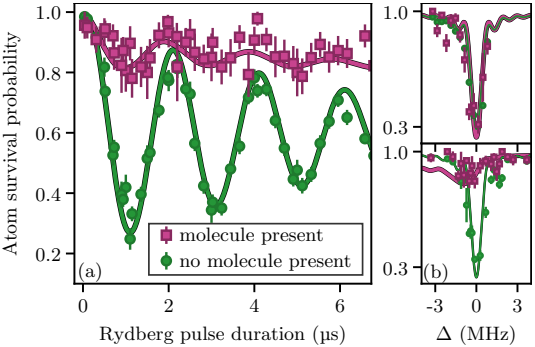


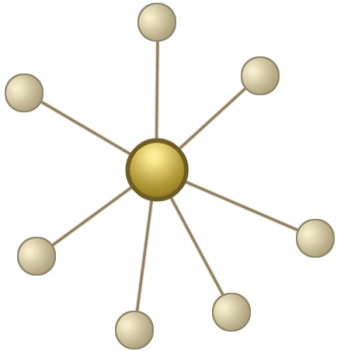


Rydberg blockade due to the charge-dipole interaction

The central spin model with a **Rydberg atom** and **polar molecules** in optical tweezers

with Dr. Jacek Dobrzyniecki

What are central spin models?



- they describe a central spin, interacting with multiple environmental spins

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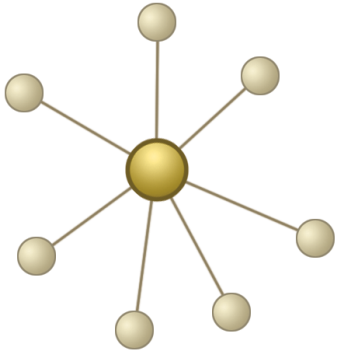

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- used to describe various realistic systems:
  - electrons in quantum dots (e.g. in GaAs) interacting with nuclear spins
  - nitrogen-vacancy centers in diamond, interacting with nearby electronic/nuclear spins

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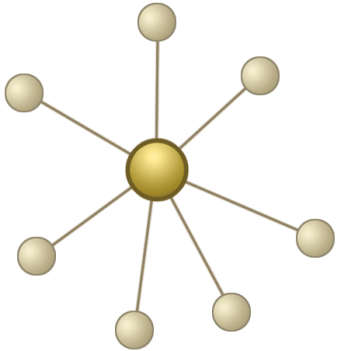

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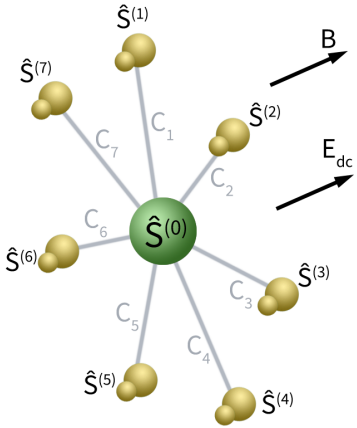
- used to describe various realistic systems:
  - electrons in quantum dots (e.g. in GaAs) interacting with nuclear spins
  - nitrogen-vacancy centers in diamond, interacting with nearby electronic/nuclear spins
- can be used to model various phenomena and processes:
  - decoherence of qubits due to environment
  - quantum sensing (e.g. detecting single nuclear spins on diamond surfaces)
  - quantum networks of connected qubits

The proposed Rydberg-molecules quantum simulator



- cold Rydberg atom and N polar molecules in desired geometry by optical tweezers

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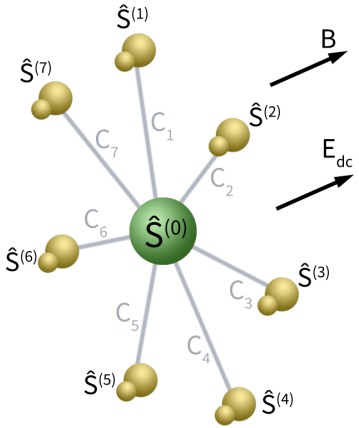

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- atom = "central 1/2-spin"
  molecules = "environmental 1/2-spins"

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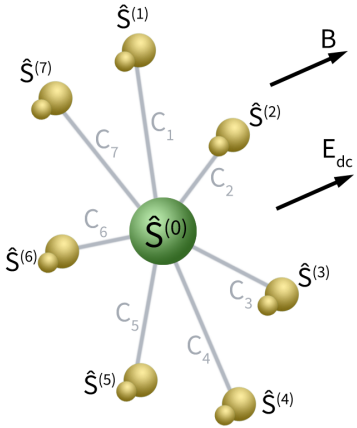

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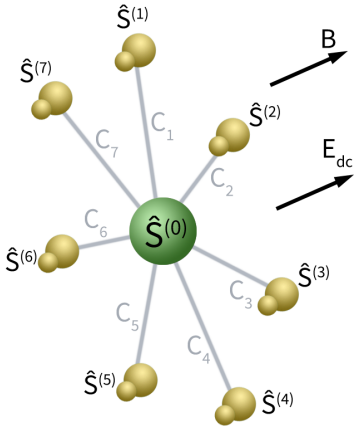

- cold Rydberg atom and N polar molecules in desired geometry by optical tweezers
- atom = "central 1/2-spin"
  molecules = "environmental 1/2-spins"
- "spin-spin" interactions by electric dipole-dipole interactions
- external magnetic and/or electric field to tune transitions into resonance

The system Hamiltonian

$$\hat{H} = \hat{h}_{\mathrm{Ryd}} + \sum_{k=1}^{N} \hat{h}_{\mathrm{mol}}^{(k)} + \sum_{k=1}^{N} \hat{V}_{\mathrm{atom-mol}}^{(k)} + \sum_{k<k'} \hat{V}_{\mathrm{mol-mol}}^{(k,k')}, \tag{1}$$

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where

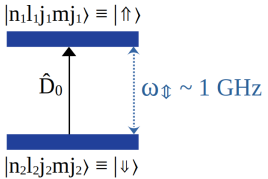
$\hat{h}_{\mathrm{Ryd}}$ – Rydberg atom single-particle Hamiltonian

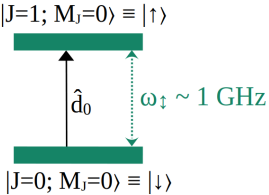
$\hat{h}_{\mathrm{mol}}^{(k)}$ – molecule single-particle Hamiltonian

$\hat{V}_{\mathrm{atom-mol}}^{(k)}$ – atom-molecule dipolar interactions

$\hat{V}_{\mathrm{mol-mol}}^{(k,k')}$ – molecule-molecule dipolar interactions

Defining the effective 1/2-pseudospin states





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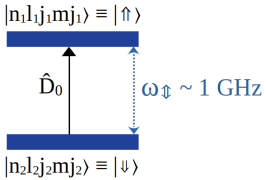
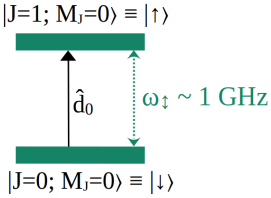


Rydberg atom ("central spin"):

- two internal atomic states $|n, l, j, m_j\rangle$ act as pseudospin states $|\Uparrow\rangle, |\Downarrow\rangle$
- $|\Uparrow\rangle, |\Downarrow\rangle$ can be coupled by electric dipole moment operators ($\hat{D}_0$, $\hat{D}_{+1}$, $\hat{D}_{-1}$)

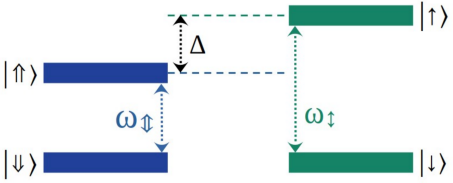


Polar molecules ("environmental spins"):

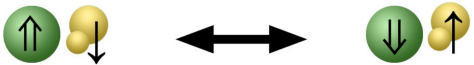
- two internal molecule states $|J, M_J\rangle$ act as pseudospin states $|\uparrow\rangle, |\downarrow\rangle$
- $|\uparrow\rangle, |\downarrow\rangle$ can be coupled by electric dipole moment operators ($\hat{d}_0$, $\hat{d}_{+1}$, $\hat{d}_{-1}$)

Matching the transition frequencies

- We set the magnetic field B to a specific value (∼100 gauss) to tune the atomic transition $\Uparrow \leftrightarrow \Downarrow$ into resonance with the molecular transition $\downarrow \leftrightarrow \uparrow$, minimizing the mismatch Δ



- When $\Delta \lesssim$ interaction strength, each molecule can resonantly exchange "spin" with the atom, through interaction of transition dipole moments



Example atom and molecule species

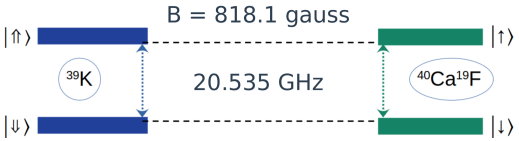
- Alkali-metal atoms: Easiest to cool and trap – obtaining singly trapped alkali-metal atoms is almost routine.

  Li, Na, K, Rb, Cs

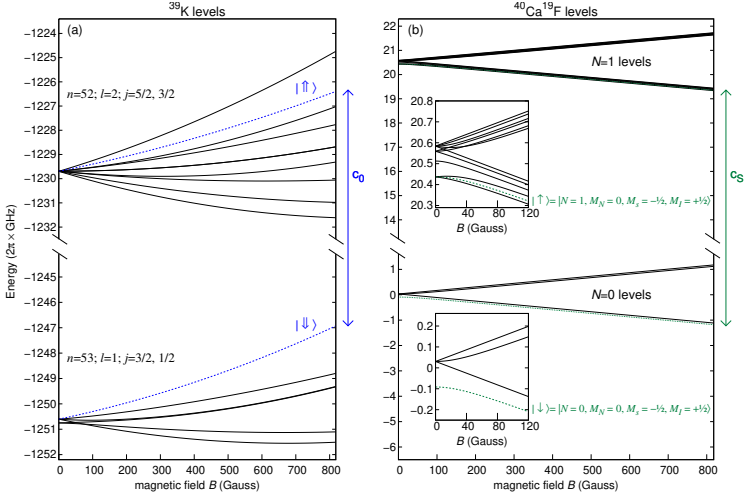
- $^2\Sigma$, $^3\Sigma$ molecules: Highly tunable with magnetic fields; already obtained experimentally in ground electronic and rovibrational states, as well as in desired hyperfine states.

  CaF, SrF, ...

Example combination:



Example: K+CaF



Obtaining the effective spin Hamiltonian

$$\hat{H} = \hat{h}_{\mathrm{atom}} + \sum_{k=1}^{N} \hat{h}_{\mathrm{mol}}^{(k)} + \hat{V}_{\mathrm{atom-mol}} + \hat{V}_{\mathrm{mol-mol}}$$

Very small in comparison with atom-molecule interactions

Obtaining the effective spin Hamiltonian

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$$\hat{h}_{\text{atom}} = \mathcal{E}_{\Uparrow} |\Uparrow\rangle\langle\Uparrow| + \mathcal{E}_{\Downarrow} |\Downarrow\rangle\langle\Downarrow|$$

$$\hat{h}_{\text{mol}}^{(k)} = \mathcal{E}_{\uparrow} \left|\uparrow^{(k)}\right\rangle \left\langle\uparrow^{(k)}\right| + \mathcal{E}_{\downarrow} \left|\downarrow^{(k)}\right\rangle \left\langle\downarrow^{(k)}\right|$$

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$$\hat{V}_{\text{atom-mol}} = \sum_{k=1}^{N} \frac{\hat{\vec{D}} \cdot \hat{\vec{d}}^{(k)} - 3\left[\hat{\vec{D}} \cdot \frac{\vec{R}_k}{|R_k|}\right]\left[\hat{\vec{d}}^{(k)} \cdot \frac{\vec{R}_k}{|R_k|}\right]}{|R_k|^3} \approx \sum_{k=1}^{N} C_k \left|\Uparrow\downarrow^{(k)}\right\rangle \left\langle\Downarrow\uparrow^{(k)}\right| + \text{H.c.}$$

(only including resonant exchange processes)

C_k depends on R_k (position of molecule k)

Effective spin Hamiltonian

Defining the effective spin operators

$$\hat{S}_z^{(k)} = \frac{|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|}{2} \qquad \hat{S}_z^{(0)} = \frac{|\Uparrow\rangle\langle\Uparrow| - |\Downarrow\rangle\langle\Downarrow|}{2}$$

$$\hat{S}_+^{(k)} = |\uparrow\rangle\langle\downarrow| = \left(\hat{S}_-^{(k)}\right)^\dagger \qquad \hat{S}_+^{(0)} = |\Uparrow\rangle\langle\Downarrow| = \left(\hat{S}_-^{(0)}\right)^\dagger$$

...The following effective spin Hamiltonian is obtained (XX central spin model / “spin star”):

$$\hat{H}_{\text{eff}} = c_T \hat{S}_z^{(0)} + c_S \sum_{k=1}^{N} \hat{S}_z^{(k)} + \sum_{k=1}^{N} \left[C_k \hat{S}_+^{(0)} \hat{S}_-^{(k)} + \text{H.c.} \right]$$

Effective spin Hamiltonian

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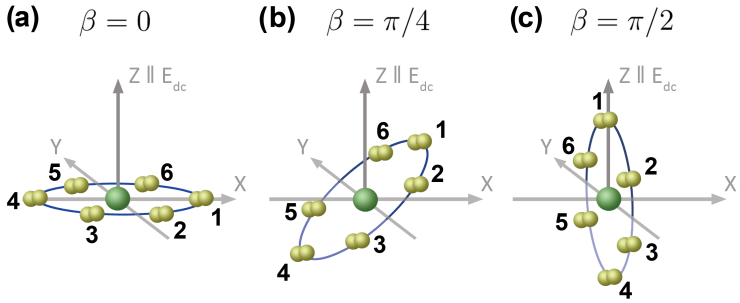
For initial states with well-defined value of total spin $\hat{S}_z^{(0)} + \sum_{k=1}^{N} \hat{S}_z^{(k)}$,

we can subtract the constant part and obtain:

$$\hat{H}_{\text{eff}} = \Delta \hat{S}_z^{(0)} + \sum_{k=1}^{N} \left[C_k \hat{S}_+^{(0)} \hat{S}_-^{(k)} + \text{H.c.} \right]$$

Example applications and dynamics

A ring-shaped geometry

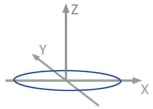


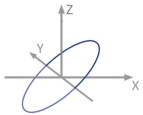
- molecules in a ring configuration
- the ring can be effectively "tilted", relative to the direction of induced dipole moments, by changing the direction of external field (which defines the Z axis)
- due to the anisotropy of dipolar interactions, the coupling constants C_k become non-uniform at tilt angles $\beta > 0$

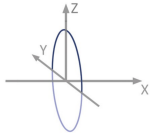
Tuning the interaction non-uniformity

Effective spin interaction arising from the dipolar interactions: $C_k \sim 1 - 3\cos^2\theta_k$

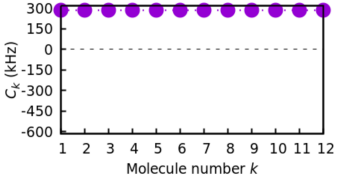
Interaction non-uniformity increases with β



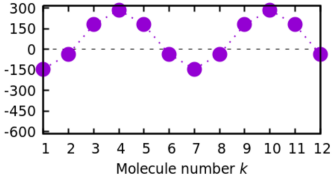




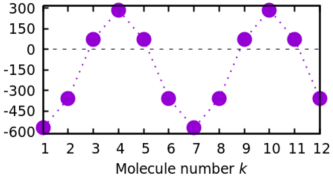
Ring tilt angle β = 0.00π



Ring tilt angle β = 0.25π

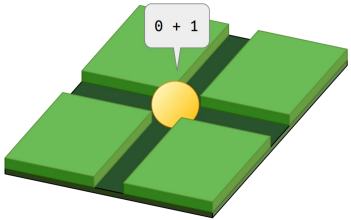


Ring tilt angle β = 0.50π



Qubit decoherence

Simulating the decoherence of a qubit,
caused by its interaction with a disordered environment



Example: an electron qubit in a quantum dot on a semiconductor surface,
interacting with the spins of surrounding nuclei

Qubit decoherence

Simulating the decoherence of a qubit,
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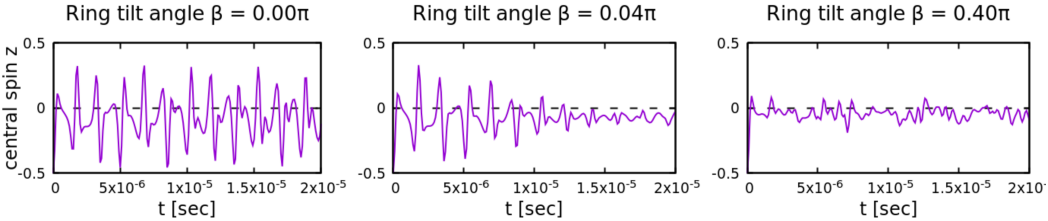
Example: an electron qubit in a quantum dot on a semiconductor surface,
interacting with the spins of surrounding nuclei

Qubit decoherence

Central spin ("qubit") dynamics in N=12 molecule system:

Initial state: $|\Downarrow\rangle\otimes|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle$

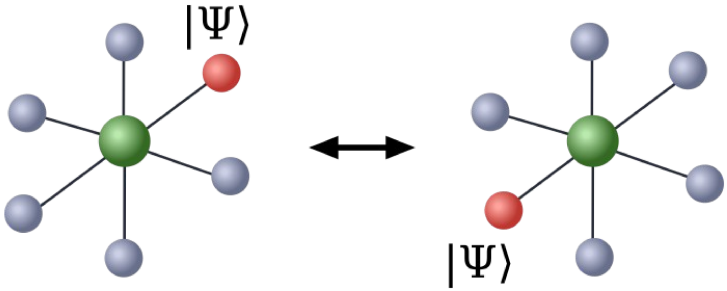


The central spin undergoes decay over time ("qubit decoherence")

Greater non-uniformity of couplings = faster decay

Timescale of the decay: $\tau \approx [\max(|C_k|) - \min(|C_k|)]^{-1}$

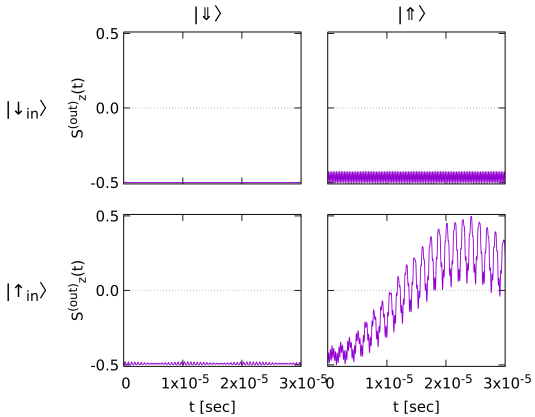
Quantum network communication



Propagating a state from one node to another in a quantum network

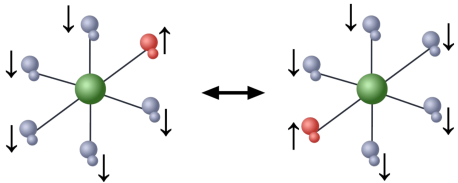
State transfer control

The initial state is $|S^{(0)}S^{(\mathrm{in})}\downarrow_2 \ldots \downarrow_8\rangle$, with $S^{(0)} = \Uparrow$ or $\Downarrow$, $S^{(\mathrm{in})} = \uparrow$ or $\downarrow$. Here the input/output spins are chosen as $S^{(\mathrm{in})} = S^{(3)}, S^{(\mathrm{out})} = S^{(7)}$).



Quantum network communication

Simplified case: Transferring a classical bit between two specific environment spins



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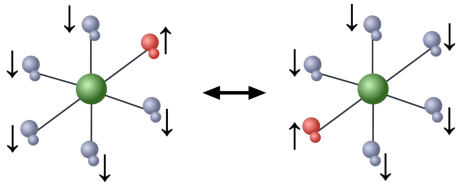
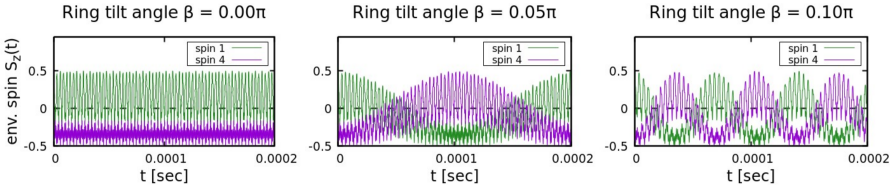


Environment spin dynamics - Initial state: N=6 molecules, $|\Uparrow\rangle\otimes|\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle$



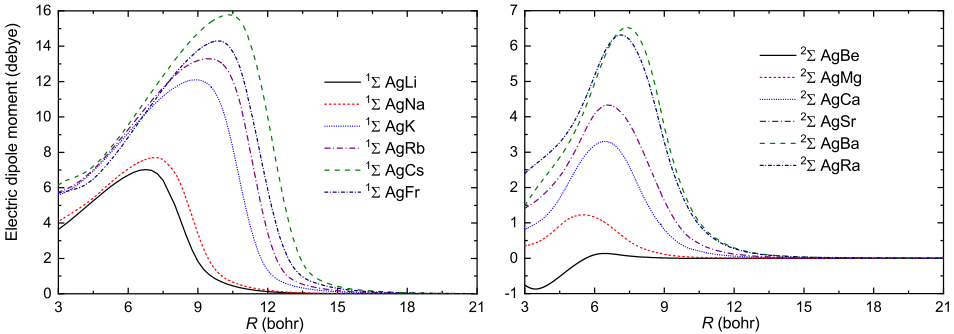
Possible extensions

What next?

- other geometries
- other field-dressing schemes
- including trap states
- highly-polar molecules (e.g. AgCs) with direct intermolecular dipolar interactions

Highly-polar molecules containing silver

M. Smialkowski, M. Tomza, Phys. Rev. A 103, 022802 (2021)



Characteristics of dipolar molecules and their intermolecular interactions

M. Smialkowski, M. Tomza, Phys. Rev. A 103, 022802 (2021)

Table: Ground-state permanent electric dipole moment d_e, polarizing electric field $\mathcal{E}_{\mathrm{pol}} = \frac{2B_e}{d_e}$, characteristic length of dipolar interaction $a_{\mathrm{dd}} = \frac{d_v^2 m}{12\pi\varepsilon_0\hbar^2}$, and characteristic nearest-neighbor energy shift $V_{\mathrm{dd}} = \frac{d_e^2}{4\pi\varepsilon_0}/(\lambda/2)^3$ for molecules in an optical lattice formed by λ =1064 nm laser.

Molecule	d_e(D)	$\mathcal{E}_{\mathrm{pol}}$ (V/cm)	a_{dd} ($10^3\, a_0$)	V_{dd} (kHz)
KAg	**8.50**	**935**	**991**	**72.4**
CsAg	**9.75**	**329**	**2144**	**95.3**
KRb	0.57	7832	4	0.3
NaRb	3.2	2594	106	10.3
LiCs	5.5	4071	398	30.3
RbSr	1.5	1467	37	2.3
CaF	3.1	13287	52	9.4

Summary

- The "XX" central spin model with a **Rydberg atom** and **polar molecules** in optical tweezers
- Example feasible implemenation in **K+CaF mixture** but applicable to other species including singlet-state alkali dimers
- The **ring-shaped** arrangement of environmental spins allows to easily tune the central-environment couplings
- Example **quantum-simulation** applications for qubit decoherence and quantum network communication

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More details: J. Dobrzyniecki, M. Tomza, **arXiv:2302.14774** (2023)

Thank you!

Workshop on Ultracold Molecules
05-08.09.2023, Warsaw, Poland
http://ultracold-molecules-2023.fuw.edu.pl