# Spin-dependent control of ultracold polar molecules in combined fields

Svetlana Kotochigova

Temple University, Physics Department,

NIST

"Fundamental Science and Applications of Ultracold Polar Molecules"
workshop
January, 2013,  KITP

# Collaborators:

Debbie Jin and Jun Ye        JILA

Dave DeMille             Yale U.

Temple U. team



Kostas Makrides



Alexander Petrov

# Ultracold ground state polar molecules

Successful creation of a near quantum degenerate gas of polar KRb and RbCs molecules in their rovibrational ground state by JILA and Innsbruck University groups opened up the possibility of studying collective phenomena, ultracold chemistry, quantum computing, and of performing precision measurements with polar molecules.



In most of these applications polar molecules are held in optical potentials, where two or more of their ro-vibrational states are manipulated and accurate measurement of transition frequency between these levels is required.
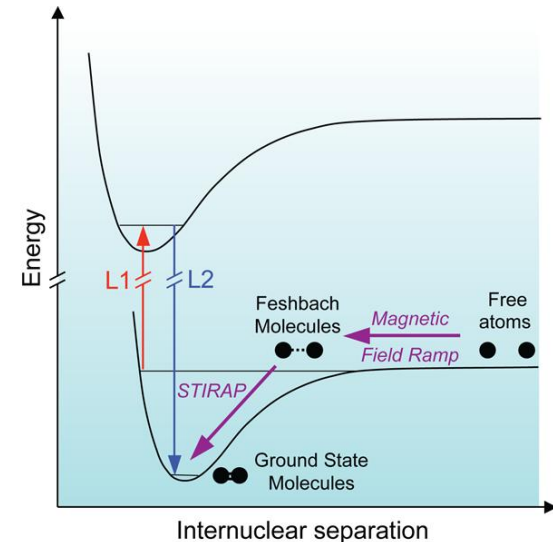
# Internal Control of Molecules

Trapping of molecules is realized by confining molecules in optical potentials

The Stark shift of these levels in the presence of trapping lasers is not exactly the same. As a result the system is sensitive to laser intensity fluctuations leading to larger measurement uncertainties (or decoherences)

Selection of trapping conditions, where internal states experience identical trapping potentials, brings substantial benefits to precision measurements and quantum computing schemes.

In the next few slides I will discuss several ways to reach this goal.

# Minimize differential Stark shifts

$$\Delta = -\alpha(\omega, \epsilon) \times I$$

Laser frequency    Polarization of light    Laser intensity

Changing frequency of trapping laser

Applying a static electric or magnetic fields

Field orientation relative to polarization of trapping light

These three results are based on "simple" model of molecule

Quantitative modeling with conditions found in JILA experiments with KRb.

The combined influence of a magnetic field, an electric field, and trapping light.

# Dynamic polarizability

The dynamic polarizability of a ro-vibrational level is due to dipole coupling to all other ro-vibrational levels and continuum states of the ground and excited potentials.

$$\alpha(h\nu, \vec{\epsilon}) = \frac{1}{\epsilon_0 c} \sum_f \frac{(E_f - ih\gamma_f/2 - E_i)}{(E_f - ih\gamma_f/2 - E_i)^2 - (h\nu)^2} \times |\langle f|d\,\hat{R}\cdot\vec{\epsilon}|i\rangle|^2.$$

Frequency    polarization    Sum $f$ over all other levels    Linewidth from spont. em.    Transition dipole moment

The multi-configuration interaction methods are used to calculate:
potential energies, permanent and transition electric dipole moments
of the molecules as a function of internuclear separation.

Calculate the dynamic polarizability $\alpha(R_e,\omega)$ as a function of $\omega$ using a couple-cluster method.
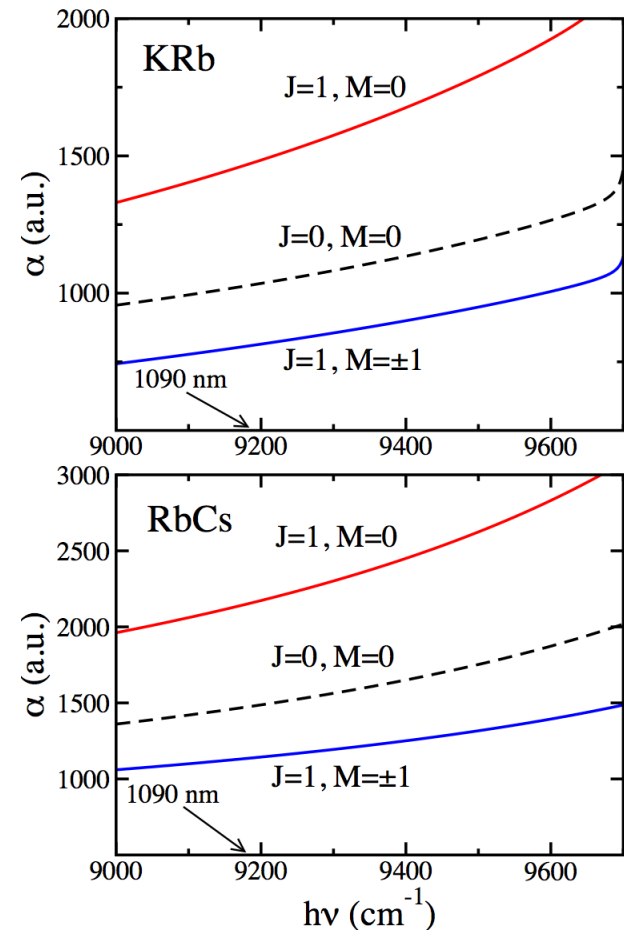
# Changing frequency

Rotating molecule with Stark shifts.

Polarizability versus laser frequency for typical trapping lasers and KRb and RbCs in their absolute lowest vibrational state.

Curves are for either J=0 or 1 rotational states and their projections M.

No crossings observed

# Applying DC electric field

Polar molecules have a permanent dipole moment and their levels can be shifted and mixed with one another by applying an external electric field. This opens up a new way to modify trapping conditions.

We extend the idea of the AC Stark shift for rotational levels to include mixing by a static electric field along a space-fixed z direction.
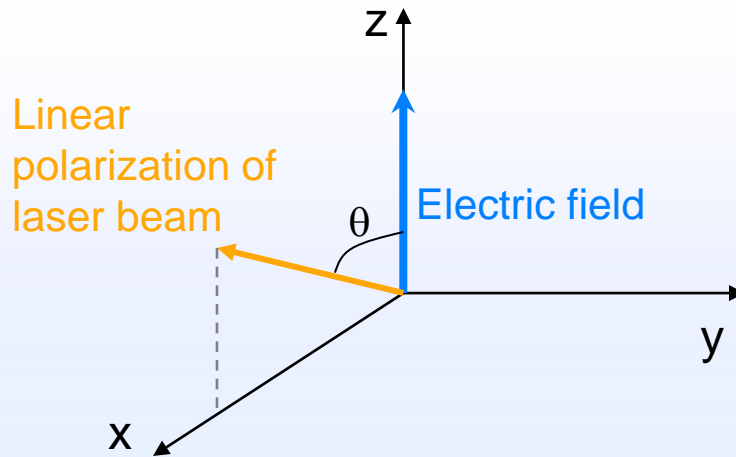
Our analyses show that the experimentally accessible electric fields mix only a few of rotational levels.



Linear polarization of laser beam

Electric field

$\theta$

z

y

x

For the external electric field strength up to 15 kV/cm, $J_{max}=10$ is sufficient for convergence.

# Magic electric field

The dynamic polarizability of the mixed rotational levels is a function of an external DC electric field and the polarization of the AC trapping field.
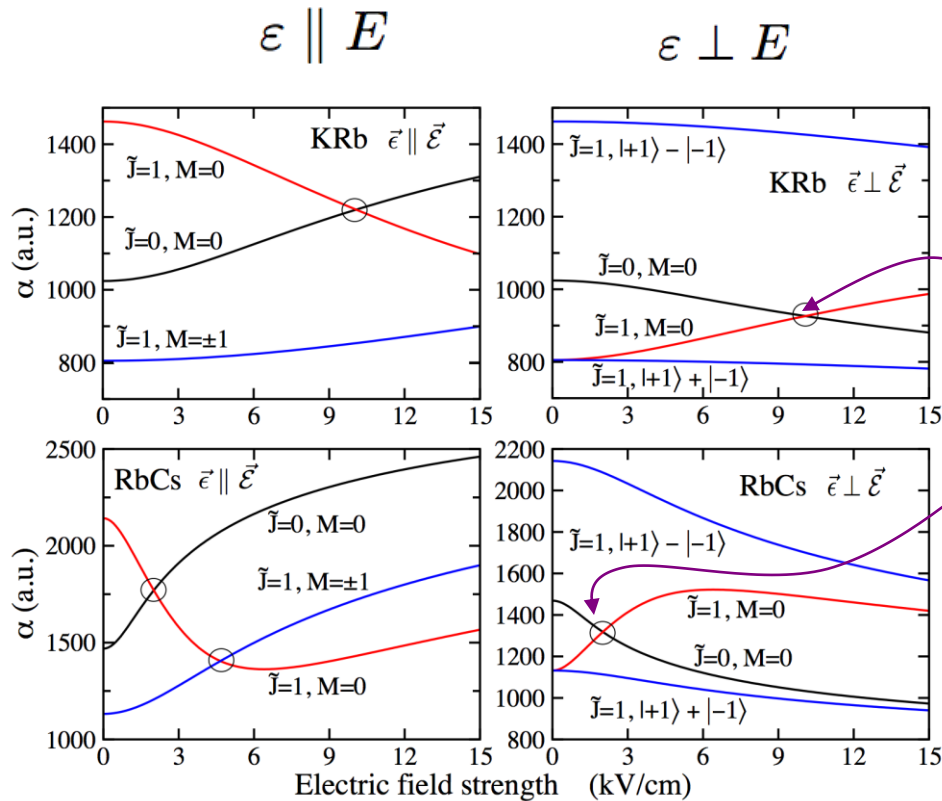


We assume a trapping laser with wavelength,

$$\lambda = 1090 \text{ nm}$$

"Magic" electric field strength (circles) can be found for pairs of J=0 and J=1 (M=0) levels at

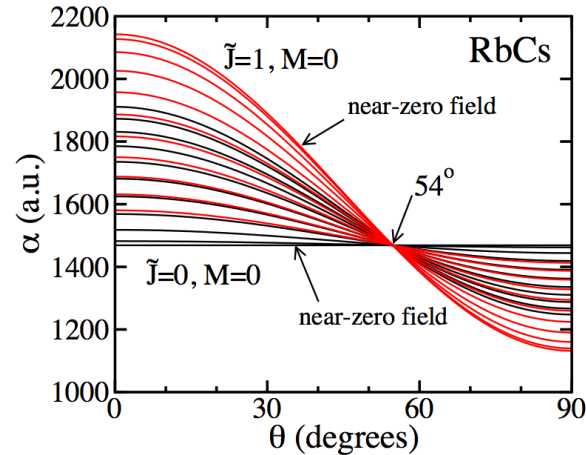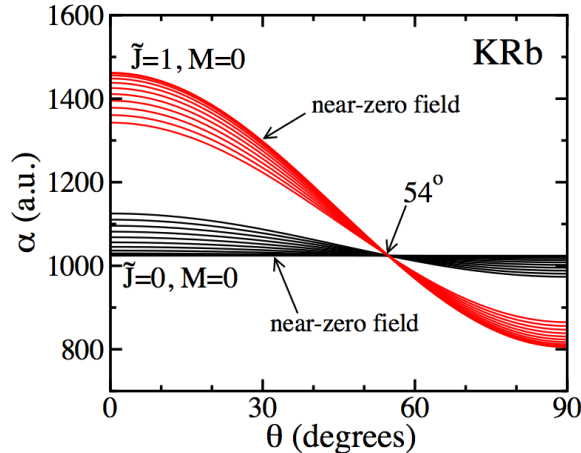10 kV/cm            for KRb
2 kV/cm and 4.6 kV/cm for RbCs.

A rather large field for KRb

# Magic Angle for M=0

Polarizability as a function of angle between E field and polarization of trapping light.

Each curve corresponds to a different electric field between

E=0-6 kV/cm                    E=0-3 kV/cm



Magic angle, where polarizability for J=0 and J=1 are equal, occurs when $\cos^2(\theta) = 1/3$ or $\theta=54^\circ$. This is consequence of the rank-2 tensor structure of the polarizability.

# Quantitative Model of JILA experiment

So far we assumed an ideal model of v=0 KRb molecules, which only included a DC electric field and the trapping field.

In reality, a magnetic field is present and an interaction between the nuclear quadrupole moments and the molecular rotation must be included.

However, there is no electric field present.

We have set up a theoretical model for the polarizability of the rotational-hyperfine levels $|JM, m_\text{K}, m_\text{Rb}\rangle$

Linear polarization of laser beam

Magnetic field

$\theta$

z

y

x

Nuclear spin projection of K and Rb
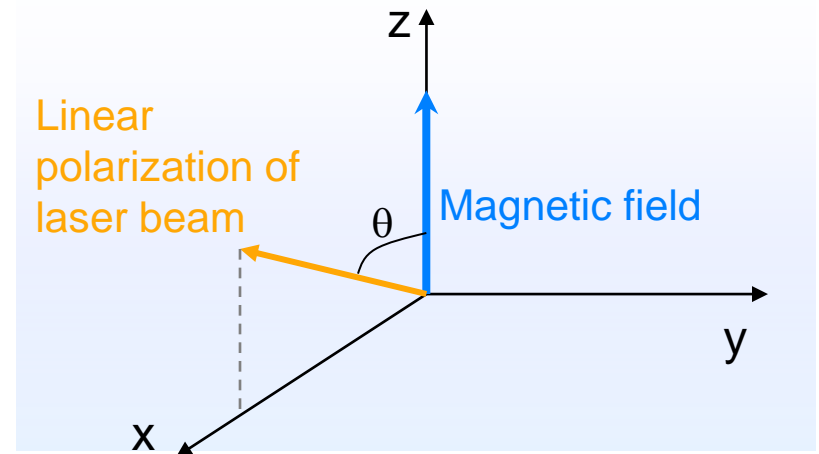
We describe their dependence on the angle $\theta$ between directions of B and $\varepsilon$.

# Exact model

The Hamiltonian for a $^1\Sigma^+$ state contains

$$B_v J(J+1)$$     rotational energy

$$-\mu_a I_{Z,a} B$$     nuclear Zeeman interaction for atom a and b

$$(eqQ)_a C_2(\theta\phi) \cdot T_2(I_a, I_a)$$     nuclear quadrupole interaction for each atom

$$-(\alpha_\parallel \mathcal{O}_\parallel + \alpha_\perp \mathcal{O}_\perp)I$$     Stark shift due to trapping potential

Hamiltonian couples 144 channels $|JM, m_{\mathrm{K}}, m_{\mathrm{Rb}}\rangle$ . The eigen states can still be identified by the channel with the largest contribution. The polarizability is determined from slope of eigen energy with respect to intensity.

In experiment we use a 1064 nm optical trap of intensity I=2.3 kW/cm$^2$ and magnetic field of 545.9 G.

We selected the eigenstates |J=0,1; M=0,+/-1; -4, 1/2> that are connected to the levels observed experimentally.

# Approximate Analytical results

Approximate Hamiltonian for the three |J=1, M=-1,0,1> rotational states, which only contains Stark shifts and quadrupole interactions.
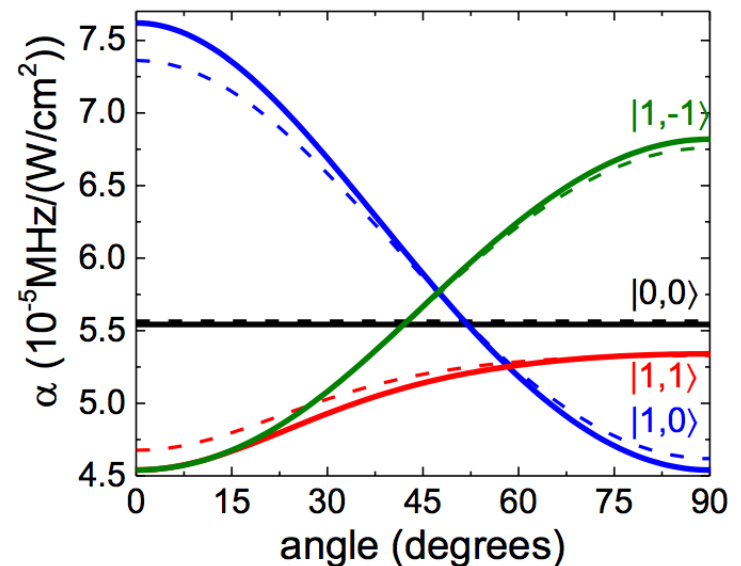
$$|1,0\rangle \qquad |1,-1\rangle \qquad |1,1\rangle$$

$$H = \begin{pmatrix} -\alpha_{11}I + \epsilon_1 & -\alpha_{12}I & -\alpha_{13}I \\ -\alpha_{12}I & -\alpha_{22}I + \epsilon_2 & -\alpha_{23}I \\ -\alpha_{13}I & -\alpha_{23}I & -\alpha_{33}I + \epsilon_3 \end{pmatrix}$$

$$\alpha_{11} = \frac{\alpha_\parallel + 4\alpha_\perp}{5}\sin^2\theta + \frac{3\alpha_\parallel + 2\alpha_\perp}{5}\cos^2\theta$$

$$\alpha_{22} = \alpha_{33} = \frac{2\alpha_\parallel + 3\alpha_\perp}{5}\sin^2\theta + \frac{\alpha_\parallel + 4\alpha_\perp}{5}\cos^2\theta$$

$$\alpha_{12} = -\alpha_{13} = \sqrt{2}\frac{\alpha_\parallel - \alpha_\perp}{5}\sin\theta\cos\theta$$

$$\alpha_{23} = \tfrac{1}{5}(\alpha_\perp - \alpha_\parallel)\sin^2\theta, \text{ depend on angle } \theta$$

comparison of analytic model with experiments
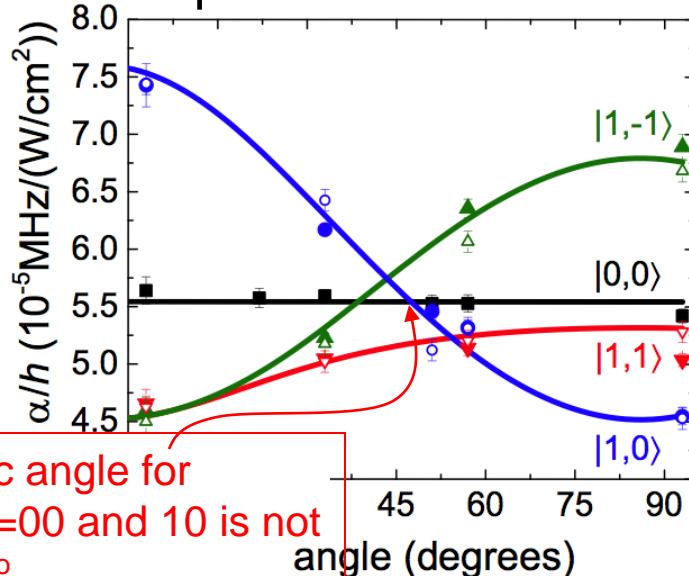
comparison of exact and analytic model. (falls within experimental error bars)



Magic angle for |JM>=00 and 10 is not at 54°

# Increase in coherence time

Experimental observation of coherence time when trapped KRb is prepared in a superposition of |J=0, M=0> and |J=1,M=0> as a function of the angle between B and polarization of trapping light.

A factor of 10 improvement is observed.



Maximum due other decoherence sources

Optimal angle
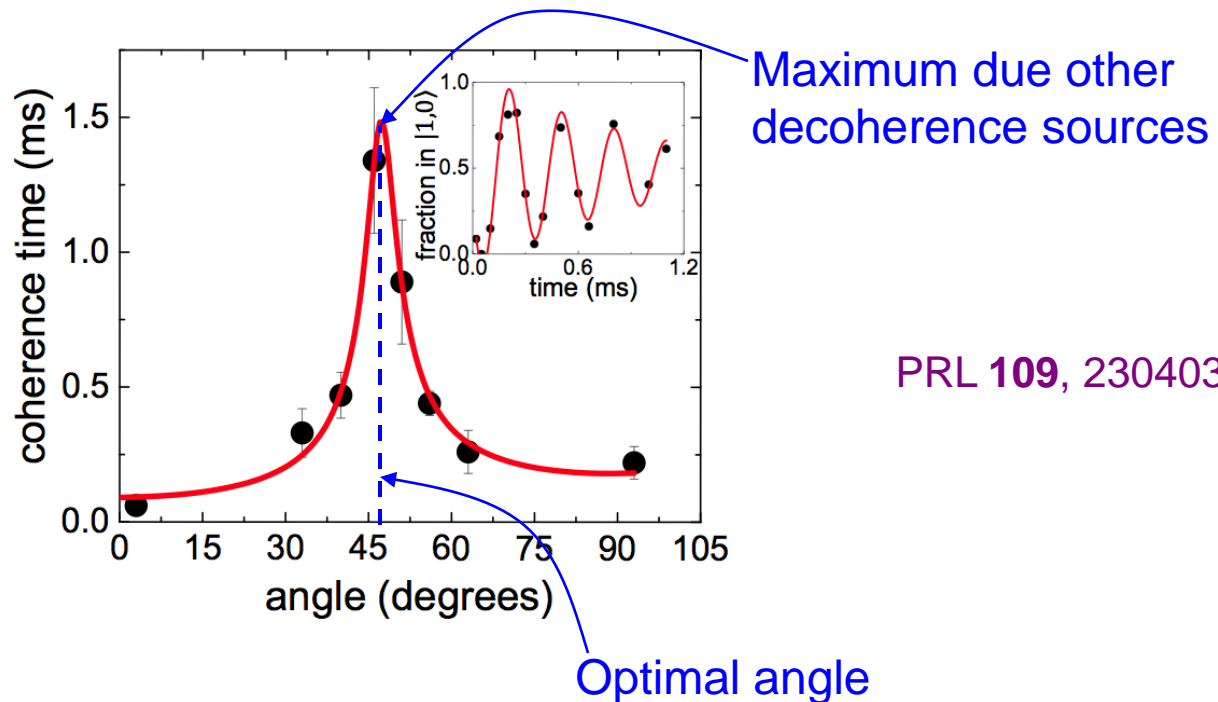
# Polar molecule in combined fields

We continue our theoretical study of the internal ro-vibronic and hyperfine quantum states when static magnetic and electric fields as well as trapping laser fields are simultaneously applied.

Understanding the effect of changing the relative orientation or polarization of these three fields is of crucial importance for creation of decoherence-free subspaces built from two or more ro-vibronic and hyperfine states.

Moreover, we evaluate the induced dipole moment of the molecule in the presence of these fields.

With the precise value of the dipole moment we will investigate interactions between molecules in different sites of an optical lattice and determine the orientation of the dipole moments.



a)

z axis

B field

E field

AC polariz.

q

j

y axis

x axis

b)
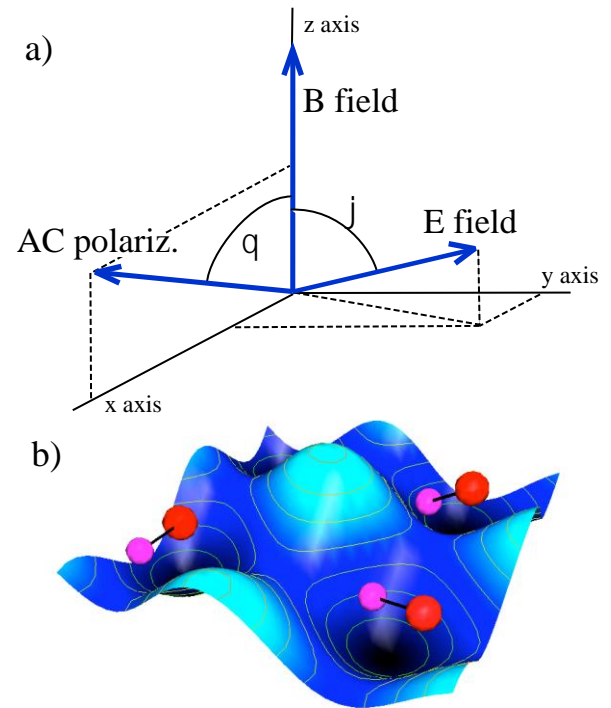
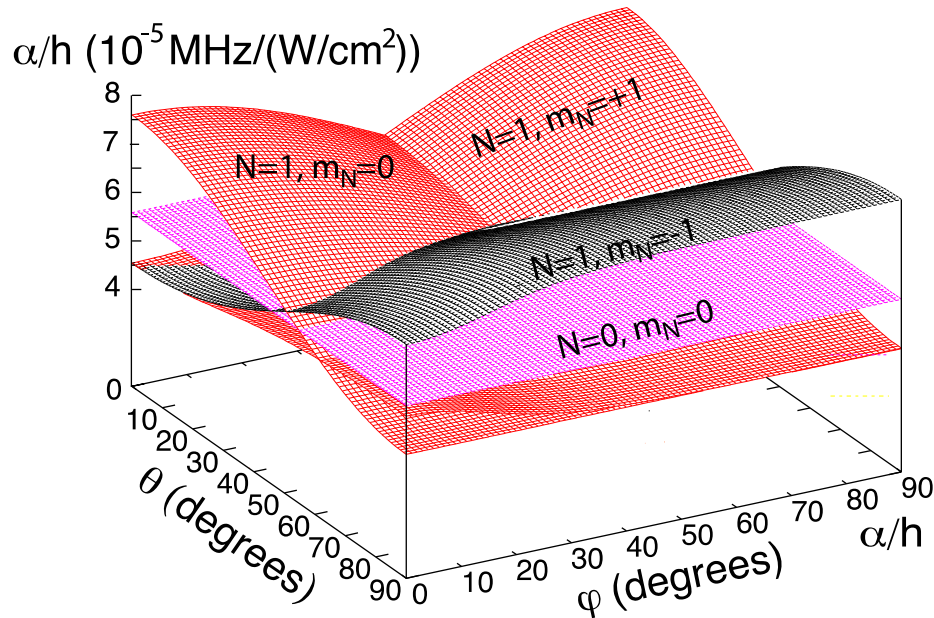# Polarizability of four rotational-hyperfine states, E=1kV/cm



Figure 1 shows that the polarizabilities of hyperfine levels coincide for many values of θ and φ angles. Crossings of polarizabilities correspond to the so-called "magic" angles θ and φ, where the differential Stark shift for two or more states is zero
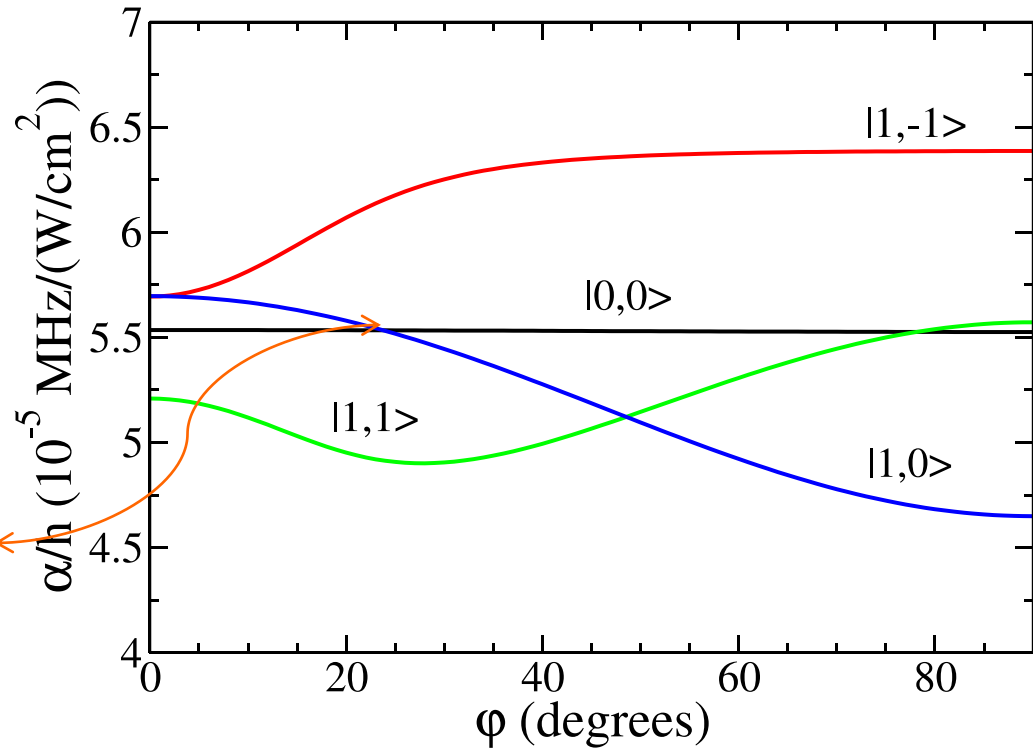
Fig. 2 shows that the magic angles between the states |0, 0⟩ and |1, 0⟩ form a nearly circular, elliptical curve that starts at θ = 57 degrees and φ = 0 degrees.
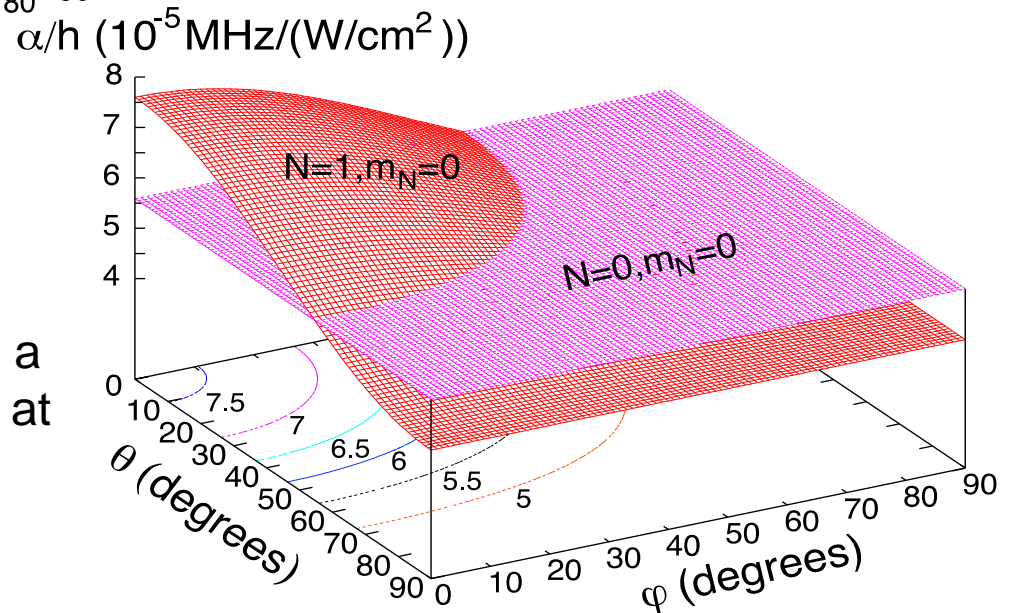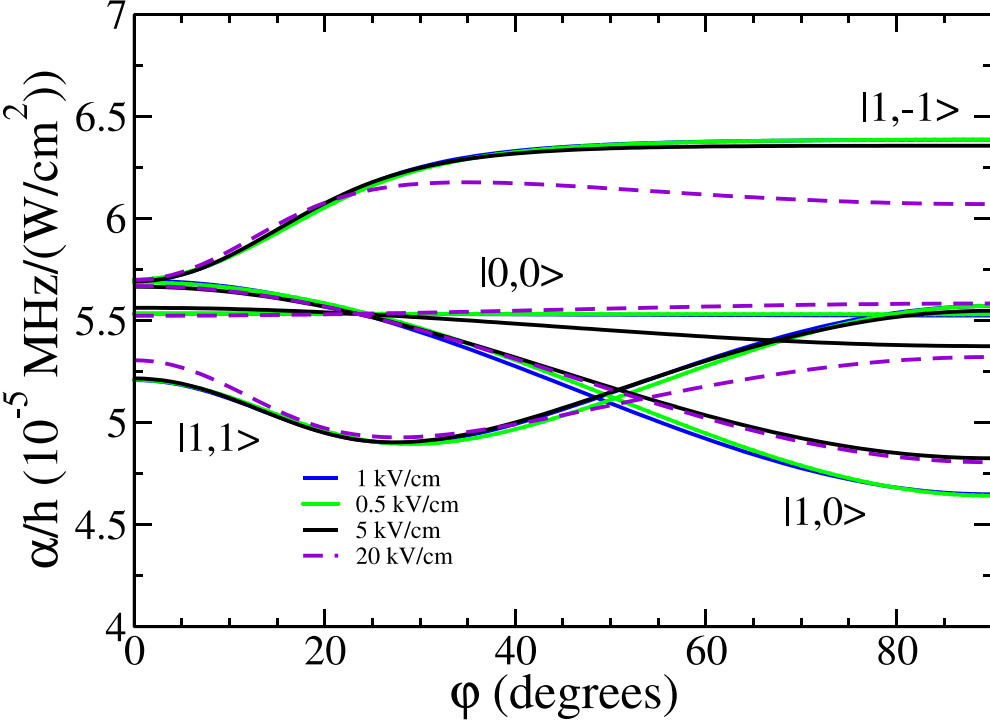
# Cut through the surfaces



E = 1 kV/cm
Θ = 51 degrees

Magic φ = 23 degrees

Conclusion: the magic conditions are sensitive to the orientation of both field.

# Large electric field strength

Magic angles do not depend on E for the large field strengths



Θ = 51 degrees

# Small field strength

Magic angles are different for the small E-field due to competition between d E and nuclear quadrupole interaction.

There is the match of the two polarizabilities over a broad range of angles.
In general, the gentler the two polarizabilities cross each other with respect to an angle the less sensitively does the rotational coherence depend on this parameter.

from 50 to 72 degrees
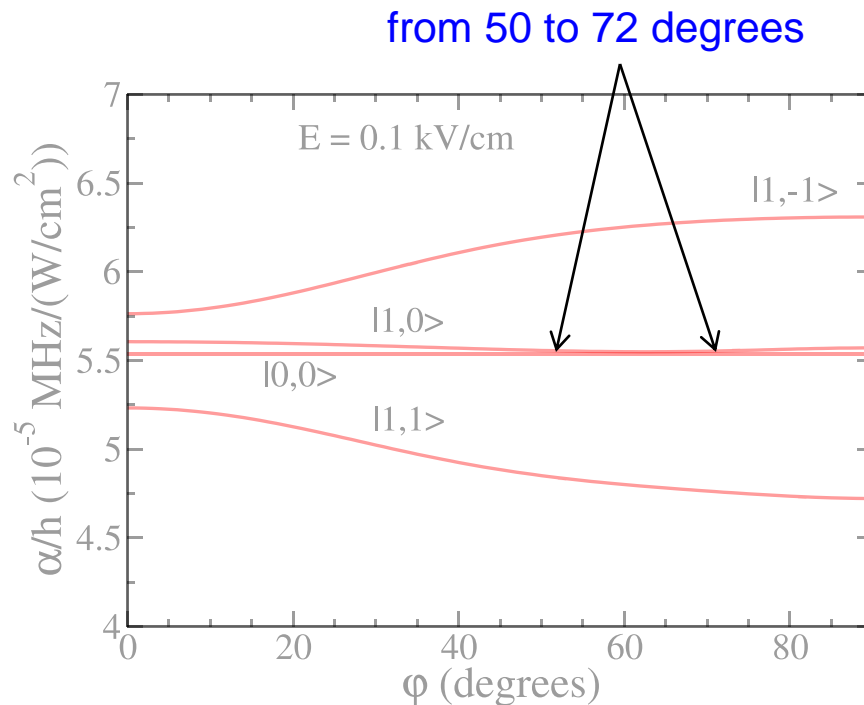
$\Theta = 51$ degrees

# Induced dipole moment
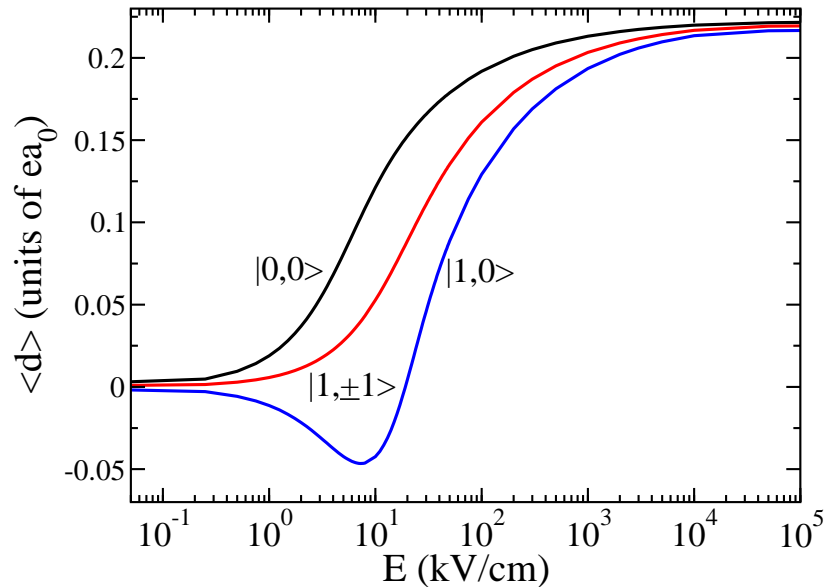


For E<7 kV/cm the dipole moment of $|1,0\rangle$ state decreases with E and is negative.

Dipole moment of $|0,0\rangle$ and $|1,\pm 1\rangle$ states always increase with E and are positive.

For $E \gg 10$ kV/cm the induced dipole moments of all four rotational-hyperfine levels converge to $d_0 = 0.223 ea_0$.

The induced dipole moment of the $|0, 0\rangle$ and $|1, \pm 1\rangle$ states have contributions from transitions to states with $N' = N + 1$ with larger rotational energies. This leads to a positive dipole moment.

For the dipole moment of the $|1, 0\rangle$ state contributions from state with both smaller and larger rotational energies appear. In this case their combined effect leads to a negative dipole moment.

# Points for discussion:

- Is E~0.1 kV/cm (small induced dipole moment) is strong enough to to be used in quantum computational schemes or simulation many-body states?

- How will interaction between polar molecules in an optical lattice will influence trapping conditions?

- What are the sources of decoherence that we need to consider in order to increase the life time of molecules in trapping potentials?