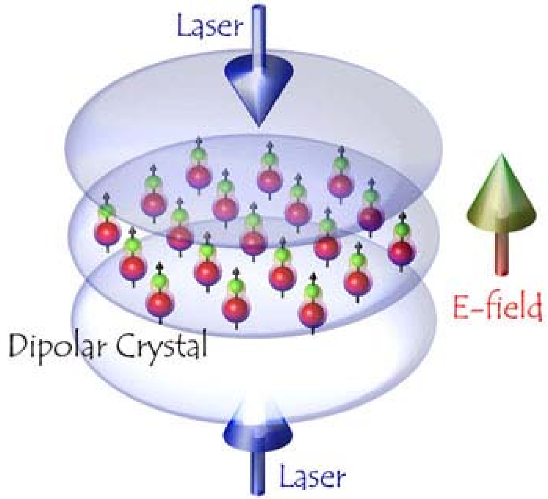
Cold Polar Molecules and their Applications for Quantum Information

H.P. Büchler

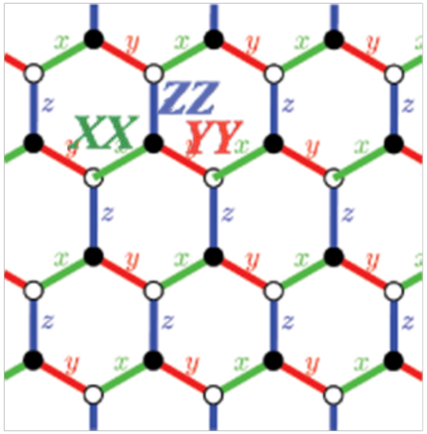
Theoretische Physik III, Universität Stuttgart, Germany

Outline



Introduction to polar molecules

- quantum melting transition between
  a crystal of and a superfluid

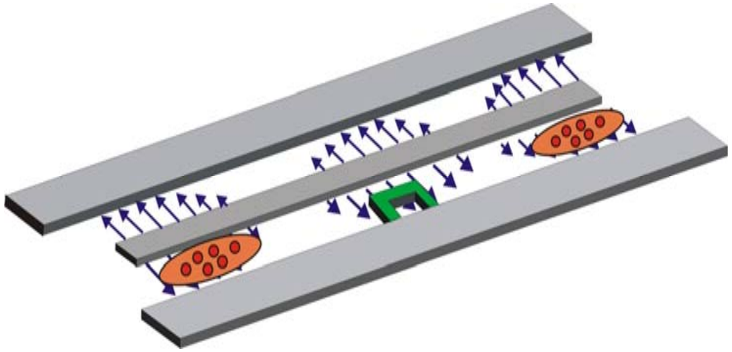


Spin toolbox

- polar molecules with spin
- realization of Kitaev model
- three-body interactions

AMO- solid state interface

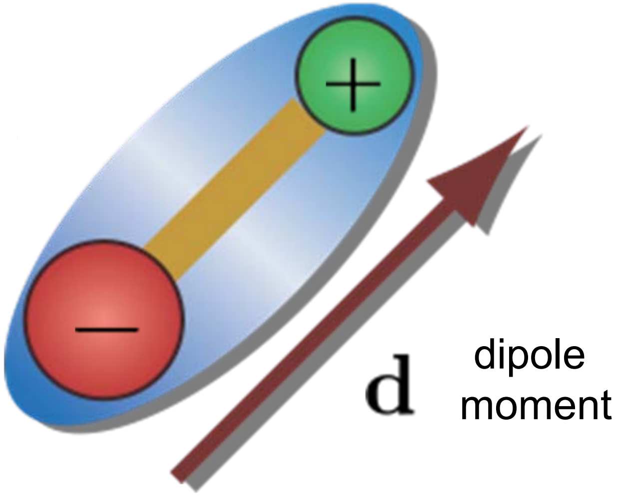
- solid state quantum processor
- molecular quantum memory



Polar molecules

Why hetronuclear polar molecules?

- coupling to optical and microwave fields
  - trapping/cooling
  - internal states
- permanent dipole moment
  - strong dipole-dipole interaction
  - long-range interaction



Polar molecules

Hetronuclear Molecules

- electronic excitations

  $\sim 10^{10}\text{Hz}$

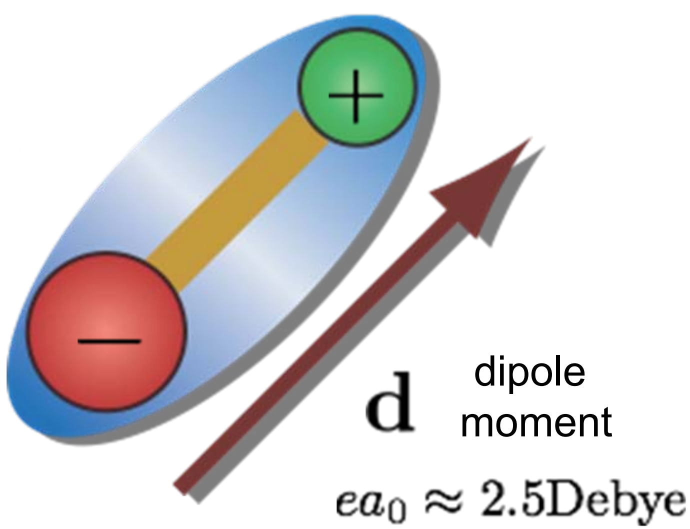
- vibrational excitations

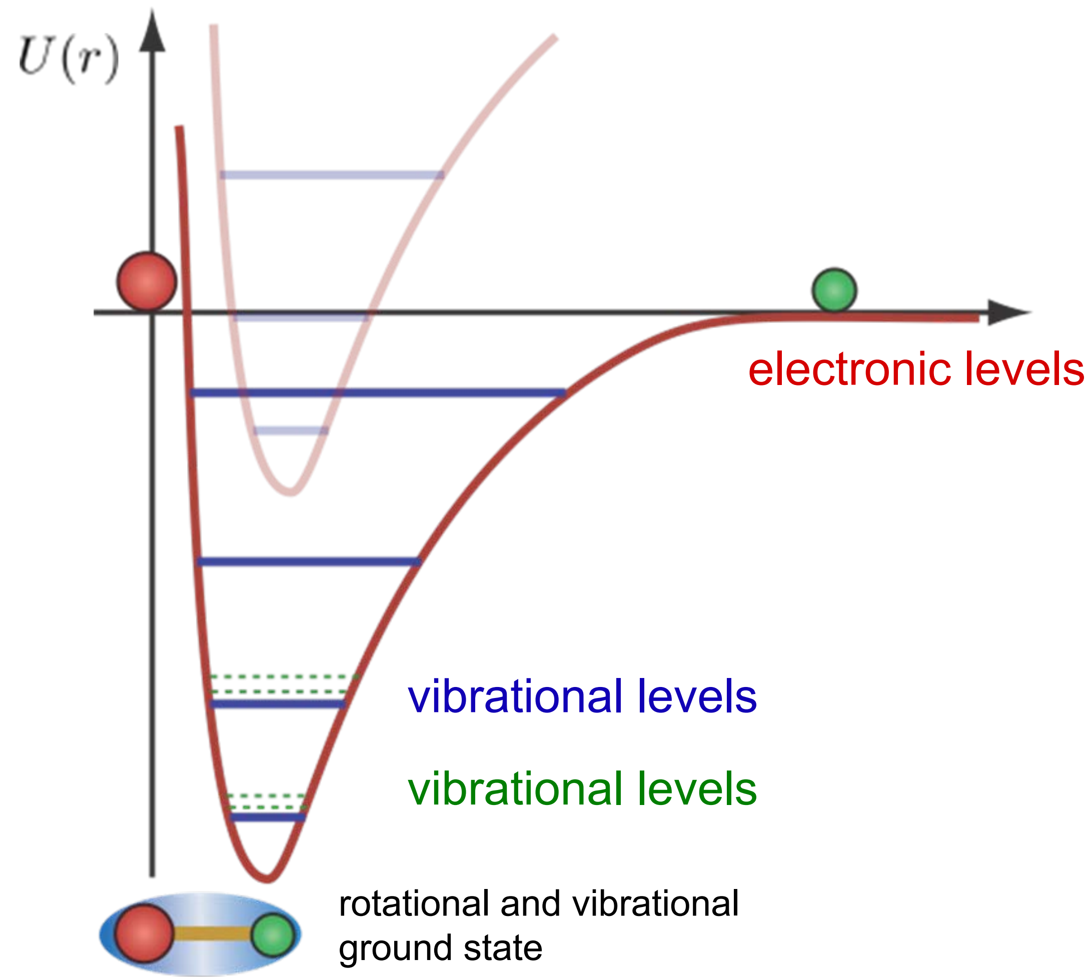
  $\sim 10^{13}\text{Hz}$

- rotational excitations (microwave fields)

  $\sim 10^{10}\text{Hz}$

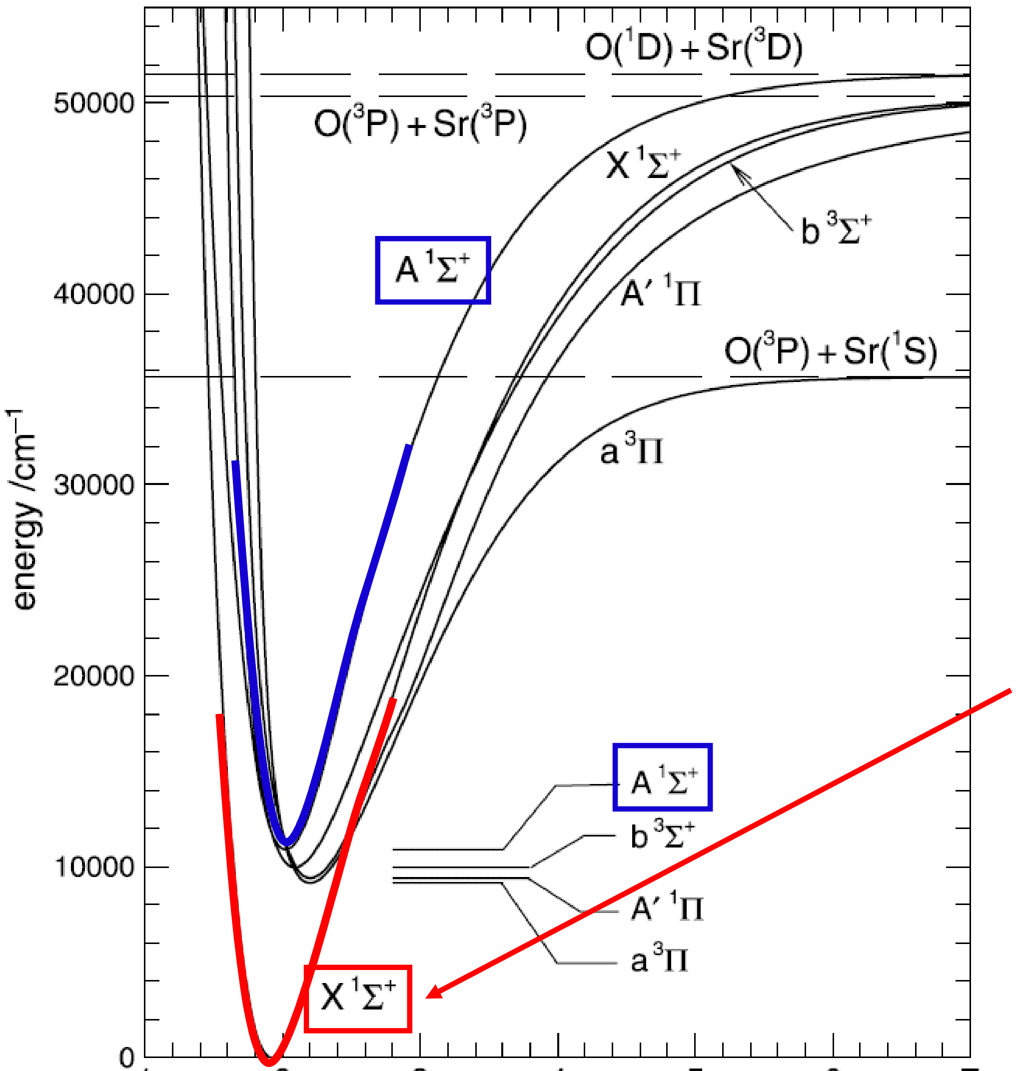
- electron spin
- nuclear spin





Polar molecule

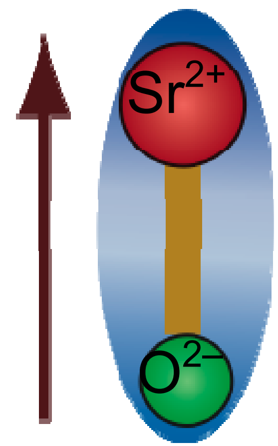
Rydberg-Klein-Rees (RKR)-potentials
(R. Skelton *et al*., 2003)



r_{eq} = 1.919 Å
d = 8.9 D

heteronuclear molecule with strong persistent dipole moment in electronic groundstate.

$Sr^{2+}O^{2-}$ ... ionic binding



$_{38}$Sr	[Kr]5s^2	
^{88}Sr	$I^p = 0^+$	(83%)
^{86}Sr	$I^p = 0^+$	(10%)
^{87}Sr	$I^p = \frac{3}{2}^+$	(7%)

$_{8}$O	$1s2s^2p^4$	
^{16}O	$I^p = 0^+$	(99.76%)
^{18}O	$I^p = 0^+$	(0.20%)

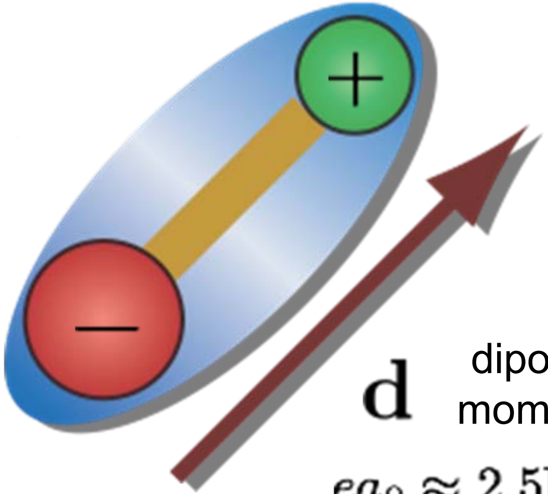
$X\ ^1\Sigma^+$ ... electronic groundstate:

S=0 ... closed shell (..$9\sigma^2\ 10\sigma^2\ 4\pi^4$)

r_{eq} = 1.919 Å ... equilibrium distance
d = 8.900 D ... dipole-moment

ω_{eq} = 19.586 THz ... vibrational const.
B_{eq} = 10.145 GHz ... rotational
I=0 ... no nuclear momenta for ^{88}SrO, ^{86}SrO

Polar molecules



$\mathbf{d}$ dipole moment

$ea_0 \approx 2.5\text{Debye}$

Polar molecules in the electronic, vibrational, and rotational ground state

- permanent dipole moment:

$$d \sim 1\!-\!9 \text{ Debye}$$

- polarizable with static electric field, and microwave fields

- interactions are increased by

$$1/\alpha^2 \sim 137^2$$

compared to magnetic dipole interactions

Strong dipole-dipole interactions tunable with external fields

$$V(\mathbf{r}) = \frac{\mathbf{d}_1\mathbf{d}_2}{r^3} - 3\frac{(\mathbf{d}_1\mathbf{r})(\mathbf{d}_2\mathbf{r})}{r^5}$$

Polar molecules

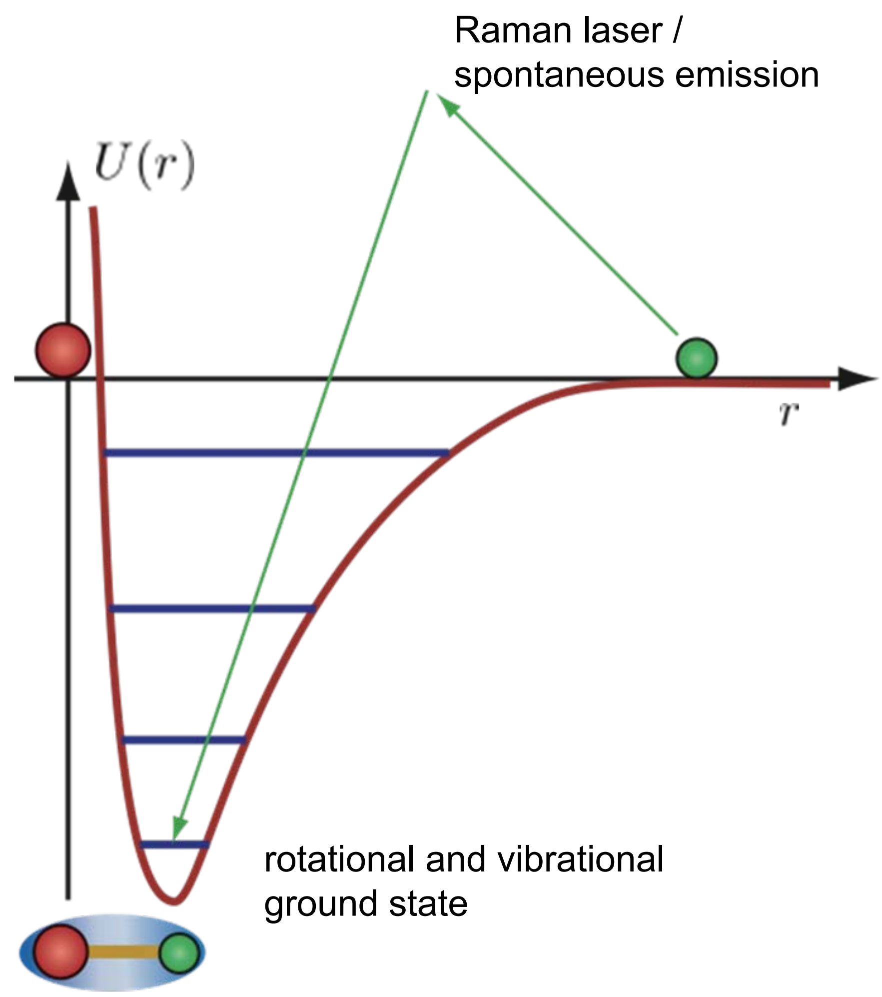
Experimental status

- Polar molecules in the rotational and vibrational ground state
- cooling and trapping techniques beeing developement:

  - cooling of polar molecules:
    D. De Mille, Yale
    J. Doyle, Harvard
    G. Rempe, Munich
    G. Meijer, Berlin
    J. Ye, JILA

  - photo association
    (all cold atom labs)

- hetronuclear molecules, e.g.,
  SrO, RbCs, LiCs, Sr F



Polar molecule

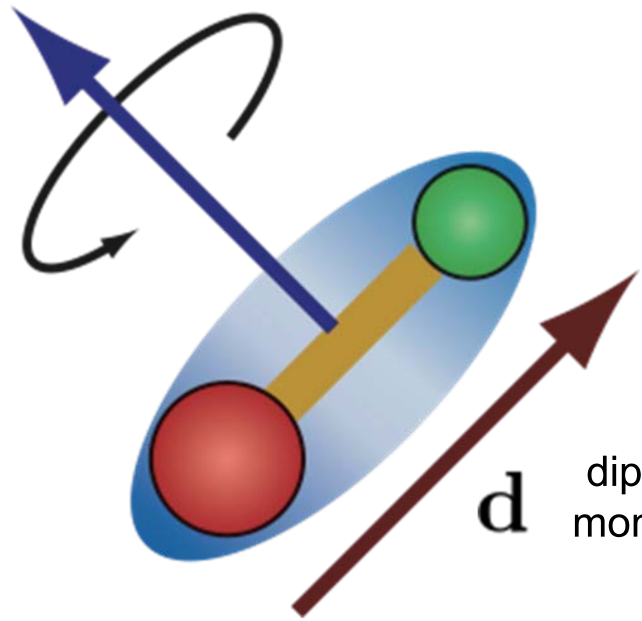
Low energy description

- rigid rotor in an electric field

$$H_{\mathrm{rot}}^{(i)} = B\mathbf{N}_i^2 - \mathbf{d}_i\mathbf{E}(t)$$

$\mathbf{N}_i$: angular momentum

$\mathbf{d}_i$: dipole operator



$BN_i(N_i+1)$

$N=0$ — — — — —

$N=1$ — — —

$N=0$ — $\Big\} \sim 20\mathrm{GHz}$

Accessible via microwave

- anharmonic spectrum
- electric dipole transition

$$\Delta N = \pm 1 \qquad \Delta m_z = -1, 0, 1$$

- microwave transition frequencies
- no spontaneous emission

Polar molecule

Dipole matrix elements

- basis states $|N, m\rangle$

- dipole operator: $d_0 = d_z$ $d_{\pm 1} = \mp(d_x \pm i d_y)/\sqrt{2}$

- matrix elements

$$\langle N+1, m+q|d_q|N, m\rangle = d\,(N, m; 1, q|N+1, m+q)\sqrt{\frac{N+1}{2N+3}}$$

Clebsch Gordan coefficient

Static electric field

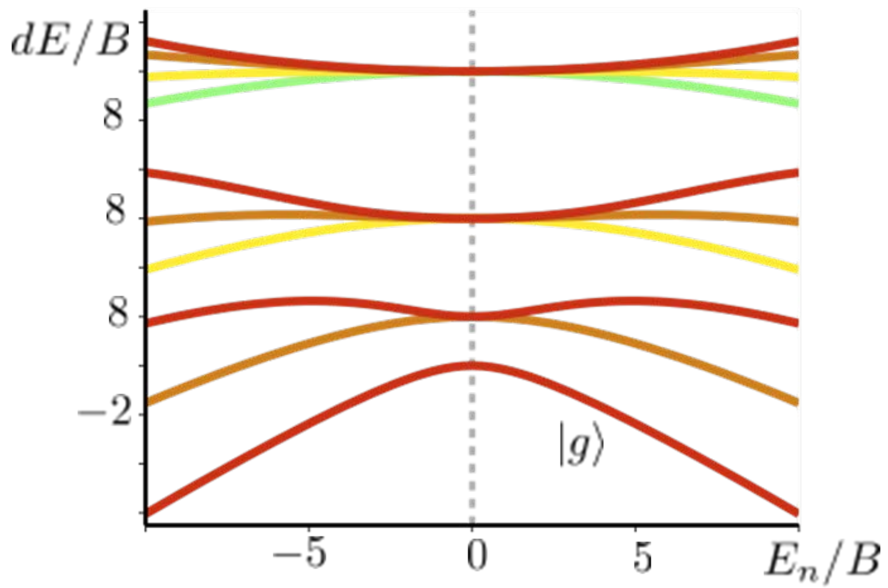
- internal Hamilton

$$H^{(i)}_{\text{rot}} = B\mathbf{N}_i^2 - \mathbf{d}_i\mathbf{E}$$

- finite averaged dipole moment

$$|\langle g|\mathbf{d}|g\rangle| = -\frac{\partial E_g}{\partial E}$$

$$D = |\langle g|\mathbf{d}_i|g\rangle|^2 \leq d^2$$

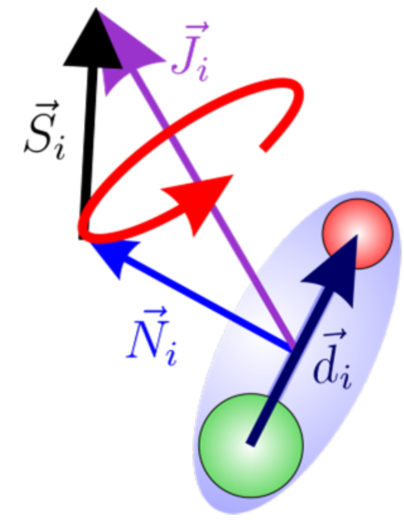


Polar molecule

Polar molecules with spin CaF

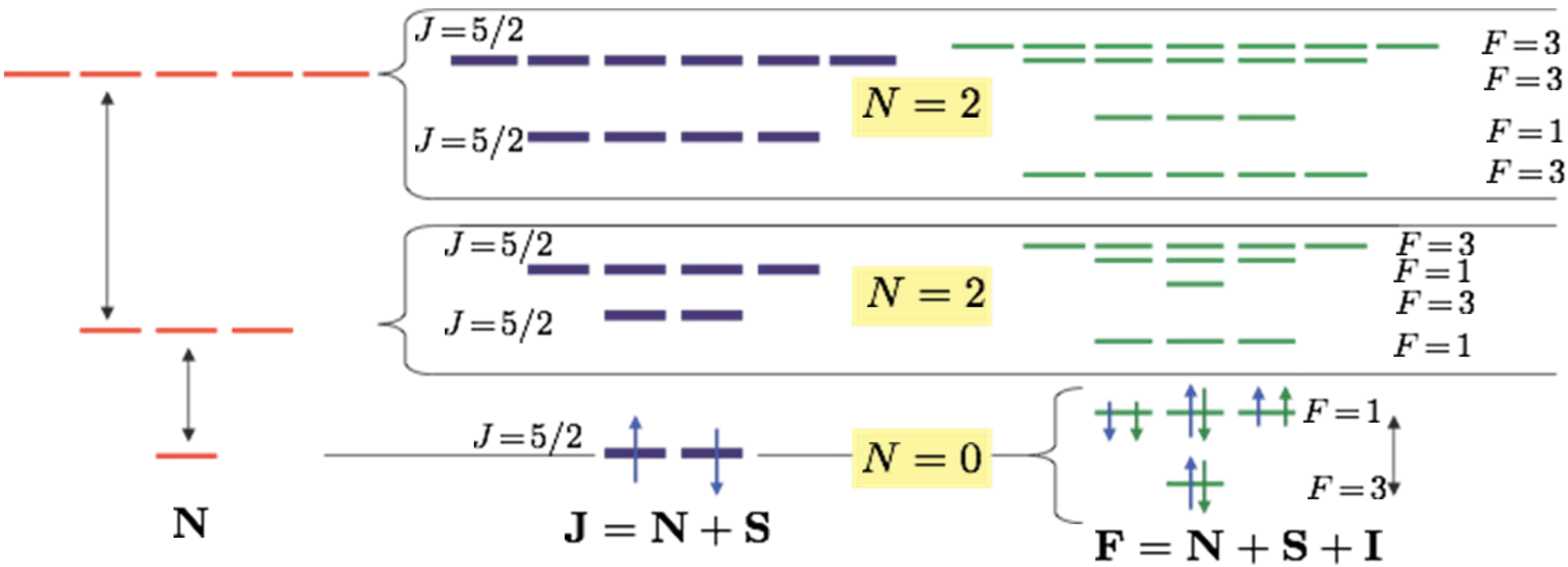
- electronic spin $S = 1/2$
- nuclear spin $I = 1/2$

spin along molecular axes



$$H = B\mathbf{N}^2 + \gamma \mathbf{N}\cdot\mathbf{S} + (b\mathbf{S}\cdot\mathbf{I} + cS_\xi I_\xi) + C\mathbf{N}\mathbf{I}$$

rigid rotor	spin-rotation	hyperfine	
$B = 10\text{GHz}$	$\gamma = 40\text{MHz}$	$b = 109\text{MHz}$	$c = 40\text{MHz}$ $C = 30\text{kHz}$



Interaction between polar molecules

Hamiltonian

$$H^{(1,2)} = \sum_{i=1}^{2} \left[\frac{\mathbf{p}_i^2}{2m} + V_{\mathrm{trap}}(\mathbf{r_i}) + B\mathbf{N}_i^2 - \mathbf{d}_i\mathbf{E} \right] + \frac{\mathbf{d}_1\mathbf{d}_2 - 3(\mathbf{d}_1\mathbf{n})(\mathbf{d}_2\mathbf{n})}{r^3}$$

kinetic energy	trapping potential	rigid rotor	electric field	interaction potential

Without external drive

- van der Waals attraction

$$V_{\mathrm{vdW}}(\mathbf{r}) = -\frac{C_6}{r^6}$$

$C_6 \approx d^4/6B$

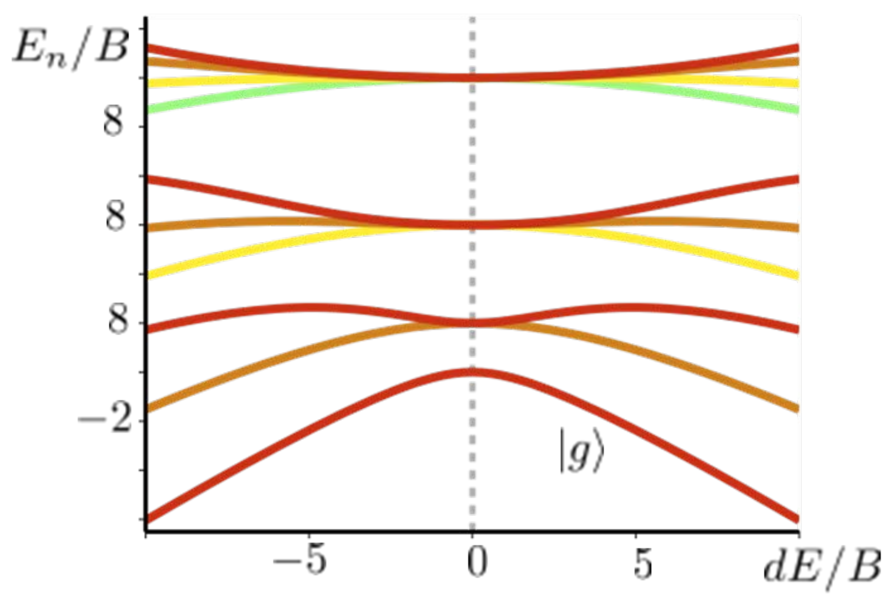
Static electric field

- internal Hamilton

$$H_{\mathrm{rot}}^{(i)} = B\mathbf{N}_i^2 - \mathbf{d}_i\mathbf{E}$$

- finite averaged dipole moment

$$D = |\langle g|\mathbf{d}_i|g\rangle|^2 \leq d^2$$

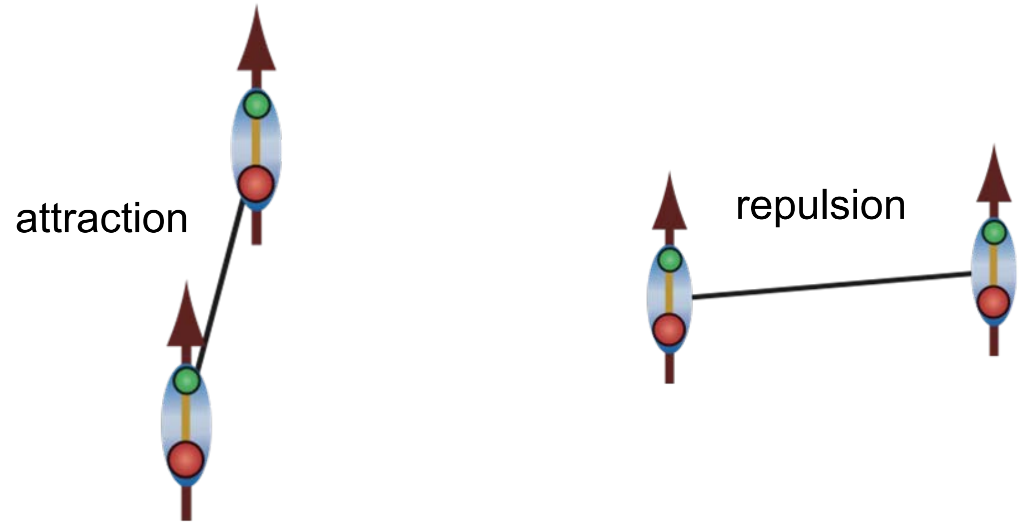


Dipole-dipole interaction

Dipole-dipole interaction

- anisotropic interaction
- long-range

$$V_{\mathrm{d-d}}(\mathbf{r}) = D\left[\frac{1}{r^3} - \frac{3z^2}{r^5}\right]$$



Weak Dipole-dipole interaction

- short-range interaction:
    - pseudo-potential
    - s-wave scattering length
- long range part via dipole-dipole interaction

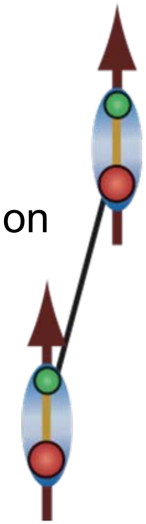
$$V(\mathbf{r}) = g\delta(\mathbf{r}) + D\left[\frac{1}{r^3} - \frac{3z^2}{r^5}\right]$$

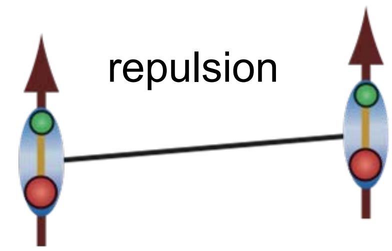
Dipole-dipole interaction

Dipole-dipole interaction

- anisotropic interaction
- long-range

$$V(\mathbf{r}) = D\left[\frac{1}{r^3} - 3\frac{z^2}{r^5}\right]$$





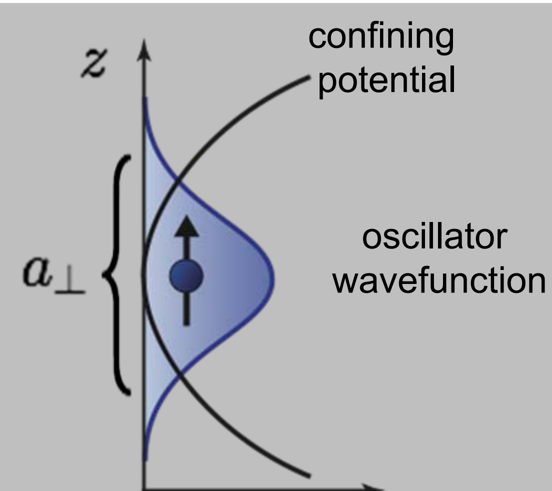
attraction ⇓

Instability in the
many-body system

- collaps of the system for increasing dipole interaction $\frac{Dm}{\hbar^2 a_s} \gtrsim 1$
  (Pfau '07)
- roton softening
- supersolids?
  (Goral et. al. '02, L. Santos et al. '03, Shlyapnikov '06)

Stability:

- strong interactions
- confining into 2D by an optical lattice



Stability via transverse confining

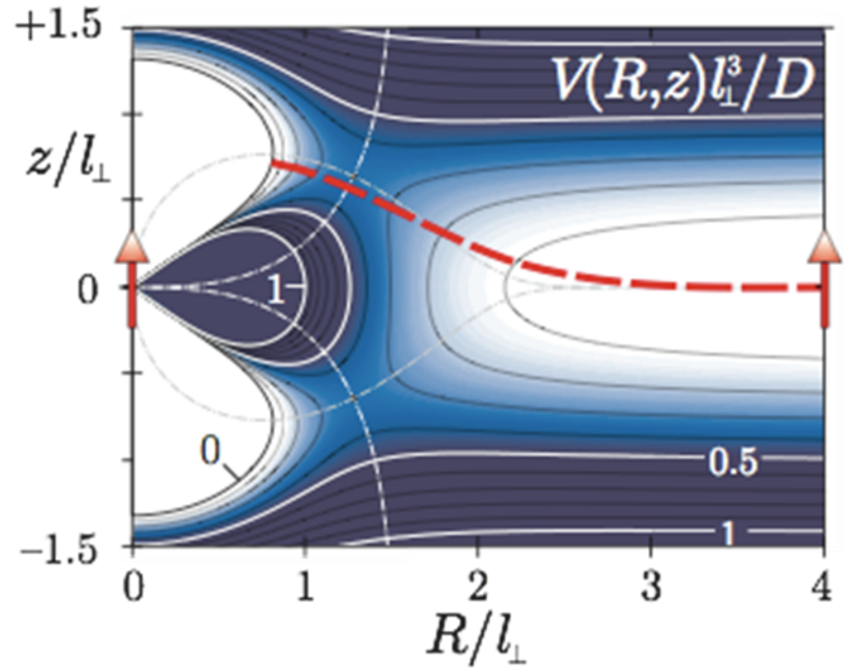
Effective interaction

- interaction potential with transverse trapping potential

$$V(\mathbf{r}) = D\left[\frac{1}{r^3} - 3\frac{z^2}{r^5}\right] + \frac{m\omega_z^2}{2} z^2$$

- characteristic length scale $\quad l_\perp = \left(\frac{Dm}{\hbar^2 a_\perp}\right)^{1/5} a_\perp$

- potential barrier: larger than kinetic energy



Tunneling rate:

- semi-classical rate (instanton techniques)

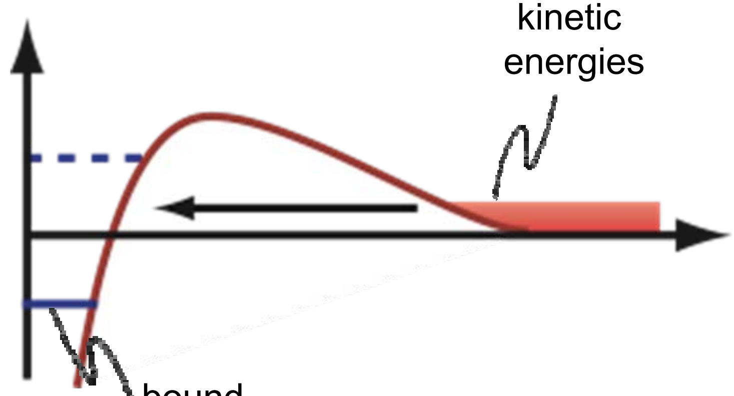
attempt frequency

$$\Gamma = A \exp\left(-S_E/\hbar\right)$$

- Euclidean action of the instanton trajectory

$$S_E = \hbar\left(\frac{Dm}{\hbar^2 a_\perp}\right)^{2/5} C$$

numerical factor: $C \approx 5.8$



Crystalline phase