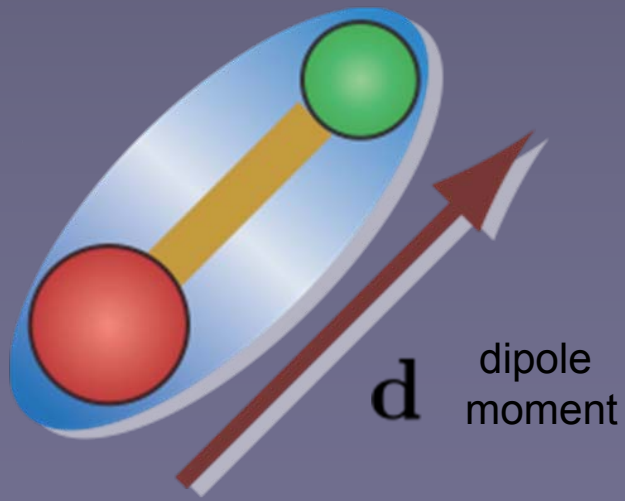
Cold Polar Molecules and their Applications for Quantum Information

H.P. Büchler

Theoretische Physik III, Universität Stuttgart, Germany



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

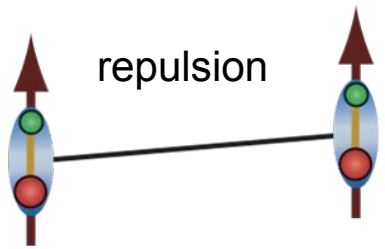
Static electric field

- internal Hamilton

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

- finite averaged dipole moment

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



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

Static electric field

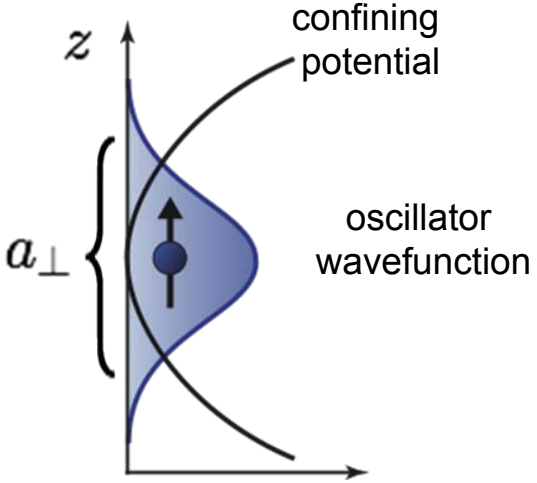
Transverse trapping

- integrating out the fast transverse motion of the molecules

transverse wave function

$$\psi(z) = \frac{1}{(\pi a_\perp^{1/4})} \exp\left(-\frac{z^2}{2a_\perp^2}\right)$$

$$V_{\rm eff}(\mathbf{R}_i - \mathbf{R}_j) = \int dz_i dz_j V(\mathbf{r}_i - \mathbf{r}_j) \left|\psi(z_i)\right|^2 \left|\psi(z_j)\right|^2$$



Effective 2D potential

- integrating out the fast transverse motion of the molecules
- large distances $|\mathbf{R}| > l_\perp$

$$V_{\rm eff}(\mathbf{R}) = \frac{D}{R^3}$$

Effective Hamiltonian

Hamiltonian

- polar molecules confined into a two-dimensional plane
- dipole interaction

interaction strength: $r_s = \frac{E_{\rm int}}{E_{\rm kin}} = \frac{Dm}{\hbar^2 a}$

$$H_{\rm eff} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \frac{D}{2} \sum_{i \neq j} \frac{1}{|\mathbf{R}_i - \mathbf{R_j}|^3}$$

Polar molecule: SrO

- dipole moment:

$\approx 4\mathrm{mK}$ $(2.4\ \mathrm{Debye} \sim e a_0)$

$r_s \sim 121 \mu m / a$

- interparticle distance: $a \sim 100 - 300\mathrm{nm}$

- stability: $S_{\rm E}/\hbar \gtrsim 130$

- transverse confining: $a_\perp \sim 40\mathrm{nm}$

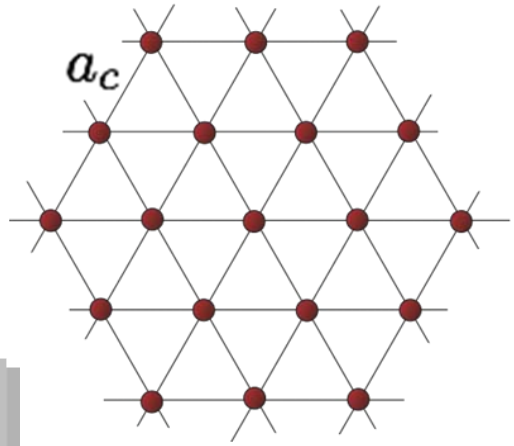
Crystalline Phase

Strong interactions

- leading order: only keep the interaction term

- describes purely classical problem

- minimization of energy: hexagonal lattice



number of particles

$$E_{\text{crystal}} = \sum_{i \neq j} V_{\text{D}}\left(\mathbf{R}_i - \mathbf{R}_j\right) = c\, N \frac{D}{a^3}$$

numerical prefactor

Lattice vibrations

- harmonic oscillations around equilibrium: phonon modes

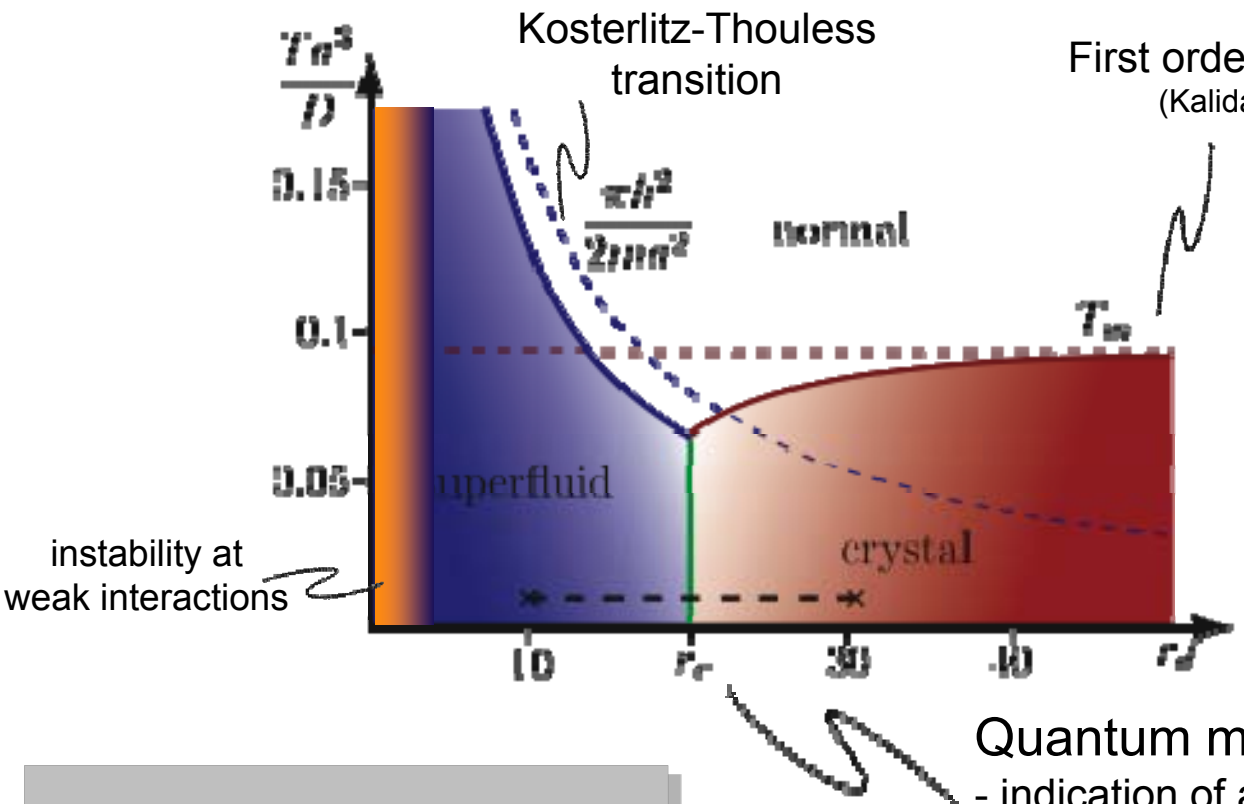
- energy correction due to zero point fluctuations of the phonons

$$E_{\text{phonon}} = \sum_{\lambda,\mathbf{k}} \hbar\omega_{\lambda,\mathbf{k}}/2 = c\frac{1}{\sqrt{r_s}}\frac{D}{a^3}$$

- lattice turns unstable to shear modes for weak transverse confining

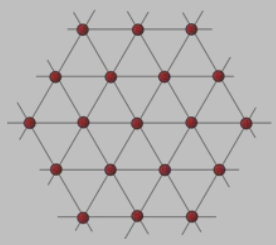
$$\gamma < \gamma_c \sim 3$$

Quantum Phase transition



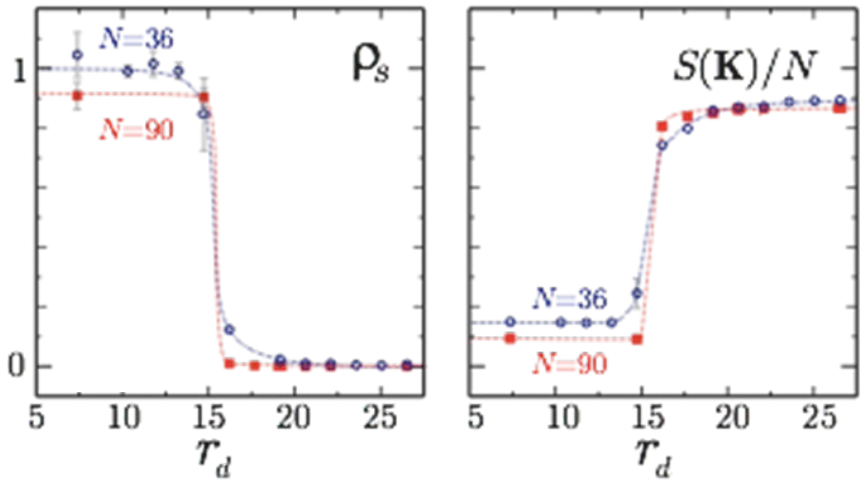
Crystal phase

- triangular lattice structure
- phonon modes



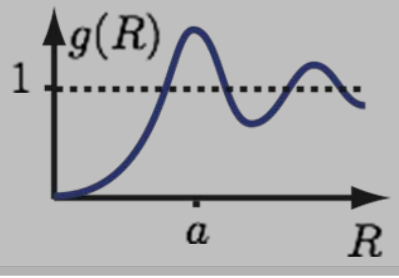
Quantum melting

- indication of a first order transition
- Quantum Monte Carlo simulations

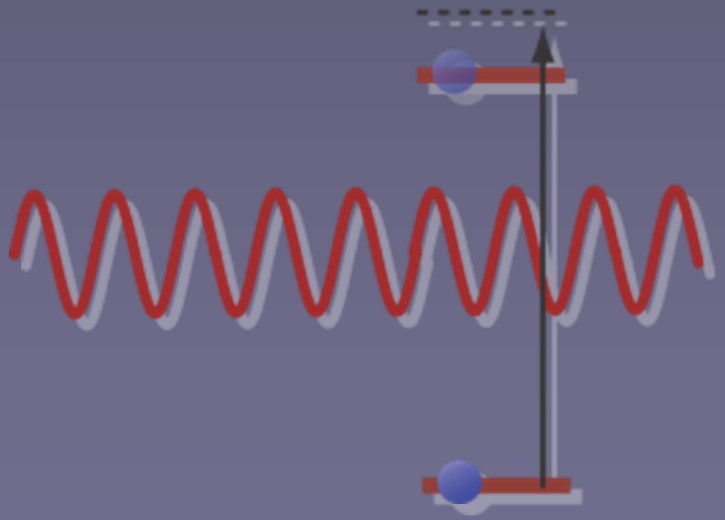


Strongly interacting superfluid

- superfluid stiffness
- large depletion



Microwave fields



Polar molecule

Low energy description

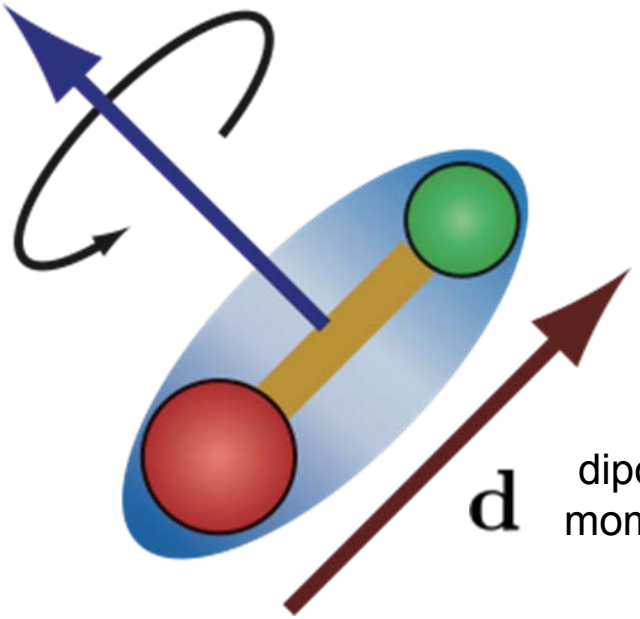
- rigid rotor in an electric field

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

$\mathbf{N}_i$: angular momentum

$\mathbf{d}_i$: dipole operator

rotation of the molecule $\mathbf{N}$



$N = 0$ — $BN_i(N_i+1)$

$N = 1$ — — —

$N = 0$ —

$\sim 20\mathrm{GHz}$

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

Single polar molecule

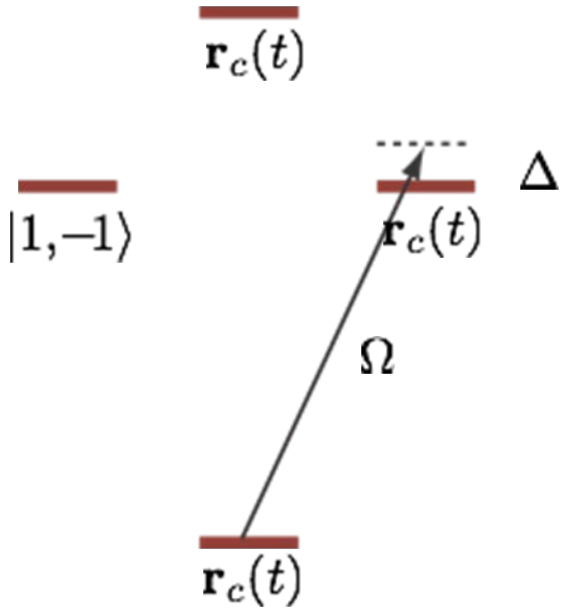
Static electric field

- along the z-axes
- splitting the degeneracy of the first excited states degeneracy
- induces finite dipole moments

$$d_g = |\langle 0,0|\mathbf{d}|0,0\rangle|$$

$$d_e = |\langle 1,1|\mathbf{d}|1,1\rangle|$$

$$d_c = |\langle 1,1|\mathbf{d}|0,0\rangle|$$



Microwave field

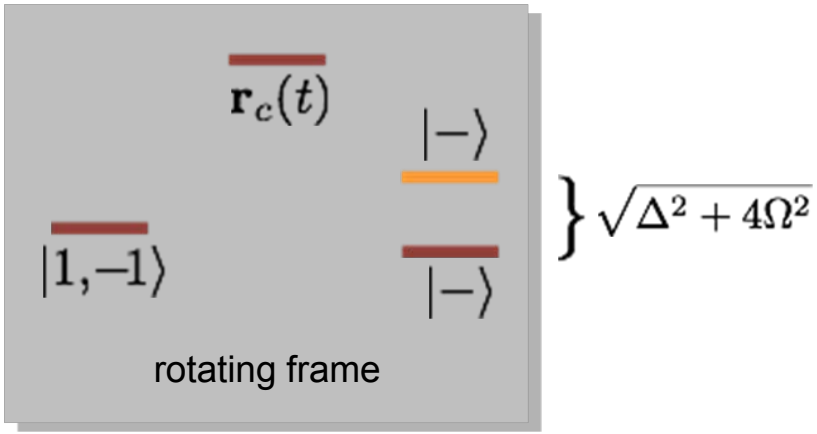
- coupling the state $|1,1\rangle$ and $|1,1\rangle$

  Δ : detuning
  Ω : rabi frequency

- rotating wave approximation
- dressed states (rotating frame)

$$|+\rangle_i = \alpha|0,0\rangle_i + \beta|1,1\rangle_i$$

$$|-\rangle_i = -\beta|0,0\rangle_i + \alpha|1,1\rangle_i$$



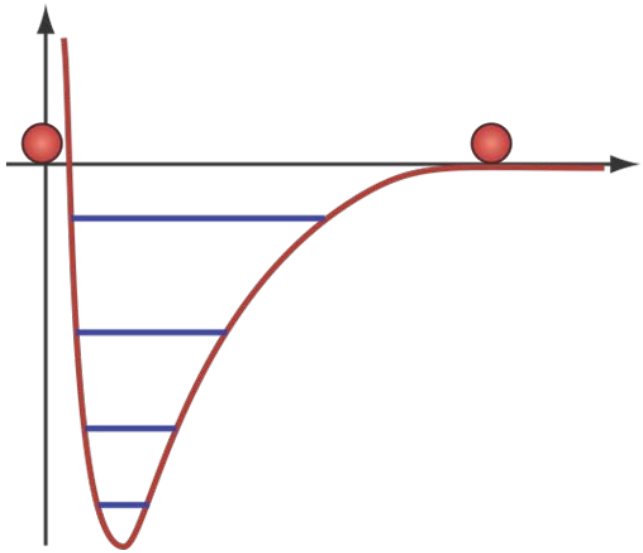
Repulsive shield

Interactions between atoms and molecules

- attractive van der Waals

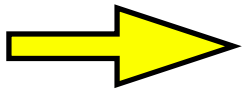
$$V_{\mathrm{vdw}}(\mathbf{r}) = -\frac{C_6}{r^6}$$

- dipole-dipole interactions



- inealstic collisions
- three-body losses
- lifetime of trapped gases
- meta-stability of cold gases

- s-wave scattering: attractive/repulsive
- Feshbach resonances



- knowledge of elastic and inelastic scattering properties
- dilute gases
- “weak” interactions

Can we trick nature?

- “blue shield” for atoms
  (see Review by Weiner *et al*, RMP 1999)

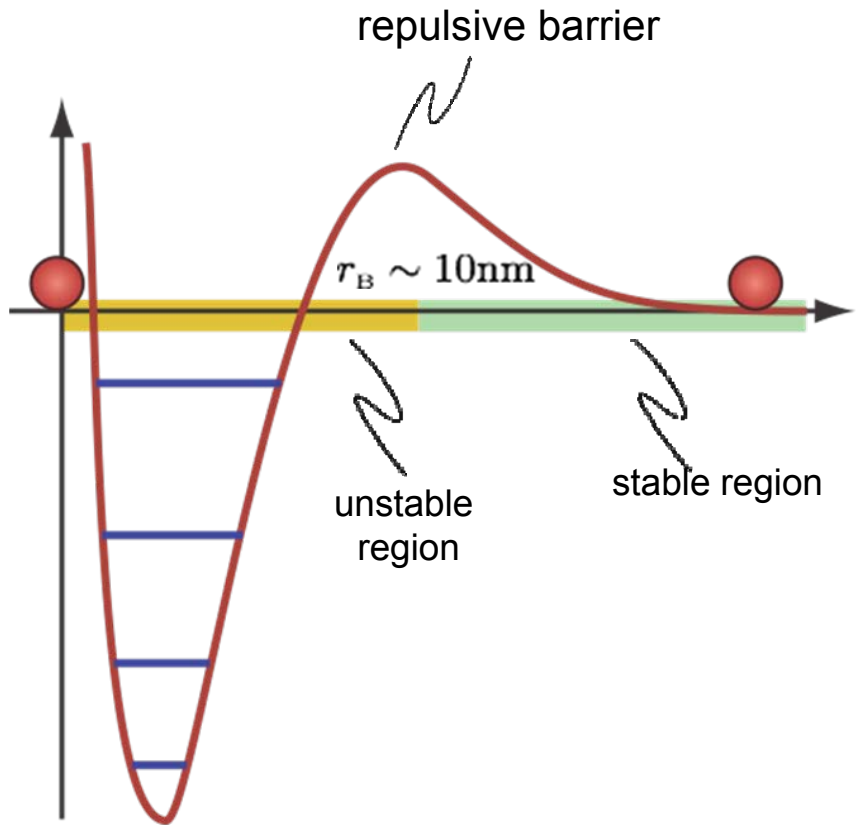
Polar molecules

Repulsive shield

- repuslive van der Waals interaction between polar molecules

- thermal activation
- quantum tunneling

→ - suppression of inelastic collisions
- large positive scattering length



Repulsive shield

Setup

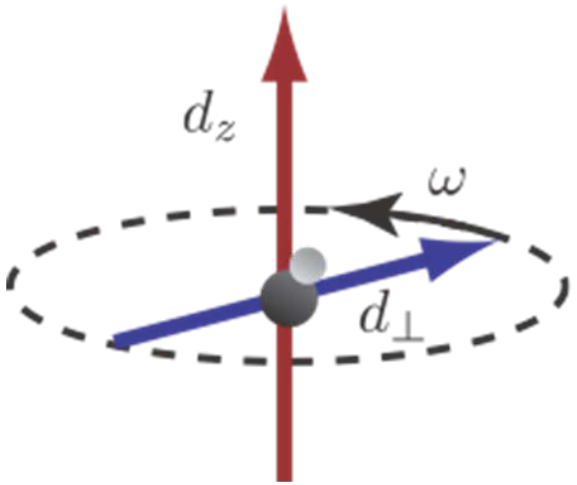
- molecules prepared into the state: $|+\rangle_i$

- dipole moment along the z-axes

$$d_z = \alpha^2 d_e + \beta^2 d_g$$

$$V(\mathbf{r}) = d_z^2 \frac{1 - 3\cos^2 s\theta}{r^6}$$

- rotation dipole moment within the plane $d_\perp = \alpha\beta d_c$

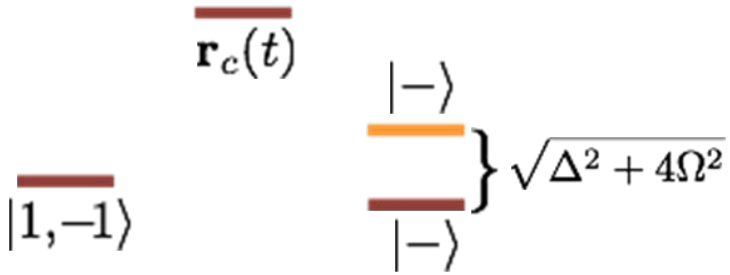


$$V(\mathbf{r}) = -\frac{d_\perp^2}{2} \frac{1 - 3\cos^2 s\theta}{r^6}$$

time averaged

- cancelation of dipole-dipole interactions

- remaining van der Waals interaction:
  repulsive and tunable



rotating frame

Born-Oppenheimer potentials

Effective interaction

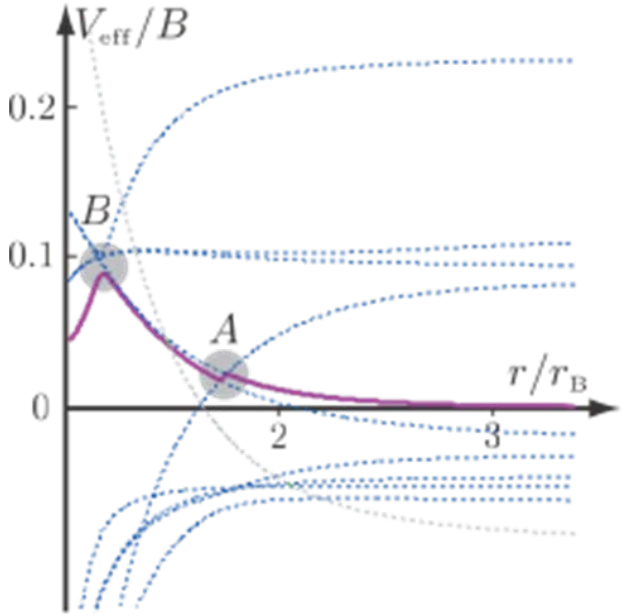
(i) diagonalizing the internal Hamiltonian for fixed interparticle distance $\mathbf{r}$.

$$\sum_i H_0^{(i)} + H_{\rm int}^{\rm stat} + H_{\rm int}^{\rm ex}$$

(ii) The eigenenergies $E(\mathbf{r})$ describe the Born-Oppenheimer potential a given state manifold.

(iii) Adiabatically connected to the groundstate

$$|G\rangle = \Pi_i |+\rangle_i$$



Length scales: $r_{\rm B} = (d^2/B)^{1/3}$

$r_\Delta = (d^2/\Delta)^{1/3}$

Repulsive shield

Long distance behavior: $r \gtrsim r_\Delta \gg r_B$

- cancelation of dipole-dipole interaction $d_\perp = d_z$

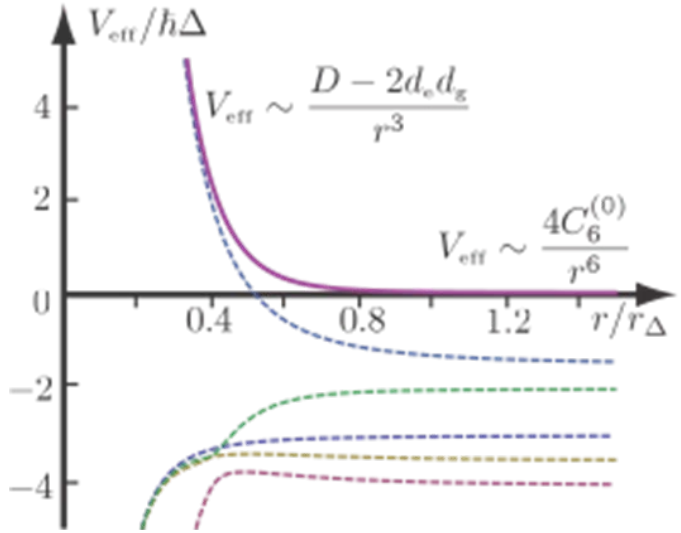
- anisotropic van der Waals repulsion

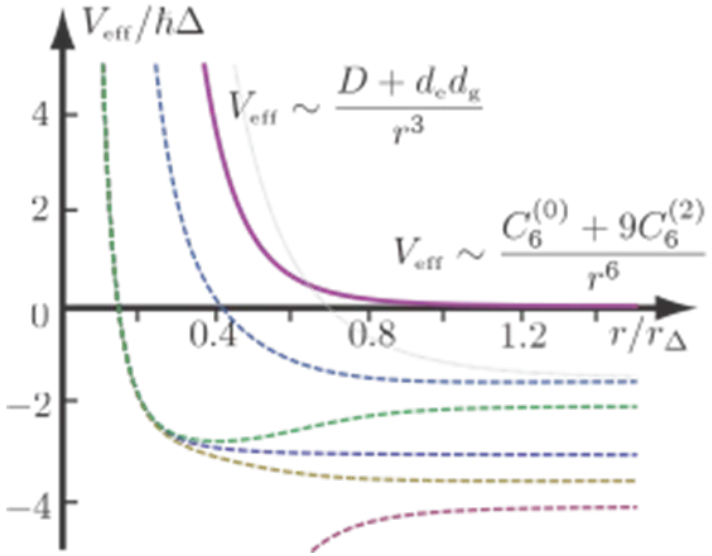
$$V_{\rm eff}(\mathbf{r}) = \frac{1}{r^6}\left[C_6^{(0)}\left(1-3\cos^2\theta\right)^2 + C_6^{(2)} 9\sin^4\theta\right]$$

$$C_6^{(0)} \approx C_6^{(2)} \sim \frac{d^4}{\Delta}$$

- crossover for $r_\Delta > r \gg r_B$

$$V_{\rm eff}(\mathbf{r}) = \frac{d_c^2 + d_g d_e\left[1-3\cos^2\theta\right]}{r^3}$$





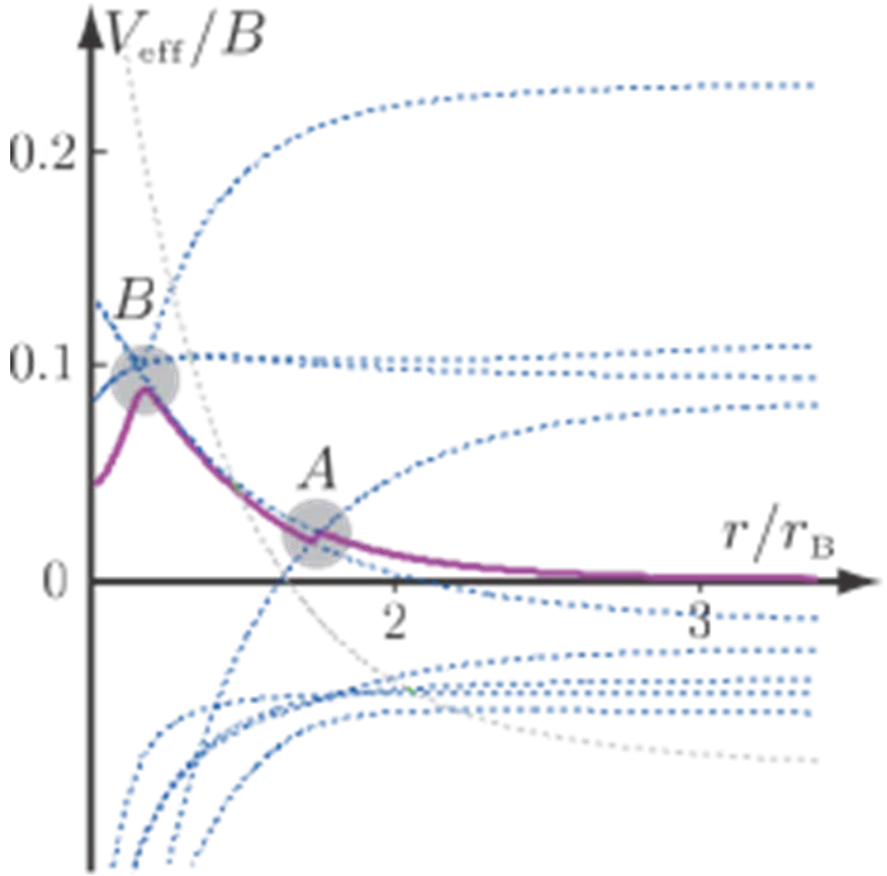
What are optimal parameters for highest possible shield?

Repulsive shield

Shorter distances $r > r_{\mathrm{B}}$

- requires to take into account all internal states

- repulsive shield is limited by the first level crossing



Optimal parameters

$dE_{\mathrm{dc}}/B = 1$: static electric field

$\Delta = 0.015B$: detuning

$\Omega/\Delta \approx 0.926$: Rabi frequency

$E_{\mathrm{shield}} \approx 0.02B$: shield barrier

$\approx 4\mathrm{mK}$: Li Cs

Repulsive shield

Validity of Born-Oppenheimer approximation:

- transitions between different levels

- mass of molecules plays an important role

$$\gamma = \frac{d^2 m}{\hbar^2 r_{\mathrm{B}}} = \frac{m\left(d^4 B\right)^{1/3}}{\hbar^2}$$

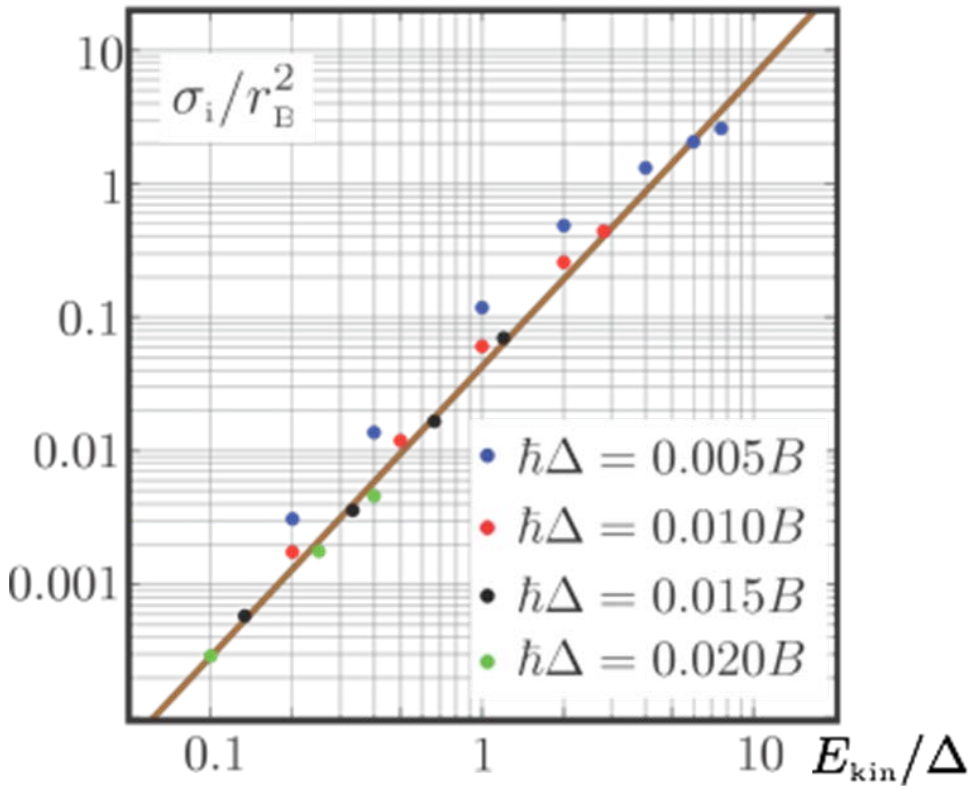
- semi-classical analysis is valid for large values of γ.

  - determine the classical motion during a collision $\mathbf{r}_c(t)$

  - full numerical solution of the Schrödinger equation for the internal states with the time-dependent position $\mathbf{r}_c(t)$

  - depletion at the turning point determines transition to different levels

Li Cs with $\gamma \approx 6900$



- algebraic behavior (no Landau-Zener like exponential behavior)

$$\sigma_{\mathrm{inel}} = \rho\left(\frac{E_{\mathrm{kin}}}{\Delta}\right)^{\kappa} r_0^2 \qquad \kappa \approx 2.2$$

$$\rho \approx 0.043$$

Repulsive shield

Quantum tunneling:

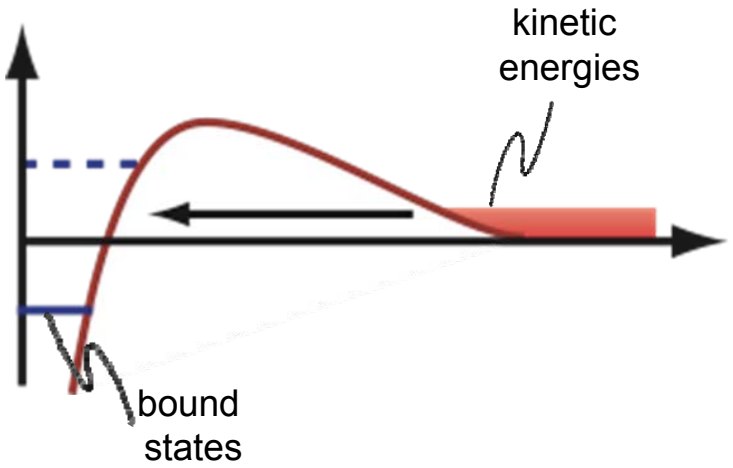
- semi-classical probablity (instanton techniques)

$$P = \exp\left(-\frac{S_E}{\hbar}\right)$$

- Euclidean action of the instanton trajectory

$$\frac{S_E}{\hbar} = 2\int_C d\mathbf{r}\sqrt{m\left[V_{\rm eff}(\mathbf{r}) - E_{\rm kin}\right]} = c\sqrt{\gamma}$$

numerical factor: $c = 0.32$



Inelastic losses

- suppressed three-body losses, as it first requires two particles to approach on short distances

- dominant loss mechanism: diabatic transitions between different levels

$$\frac{1}{\tau_{\rm ine}} \approx 10\frac{Bnr_{\rm B}^3}{\hbar}\left(\frac{T}{B}\right)^{\kappa+1/2}$$

- parameters: Li Cs

$$n \sim 10^{15}\ {\rm cm}^{-3}$$

$$T < 100\mu{\rm K}$$

$$\tau_{\rm ine} > 1{\rm sec}$$

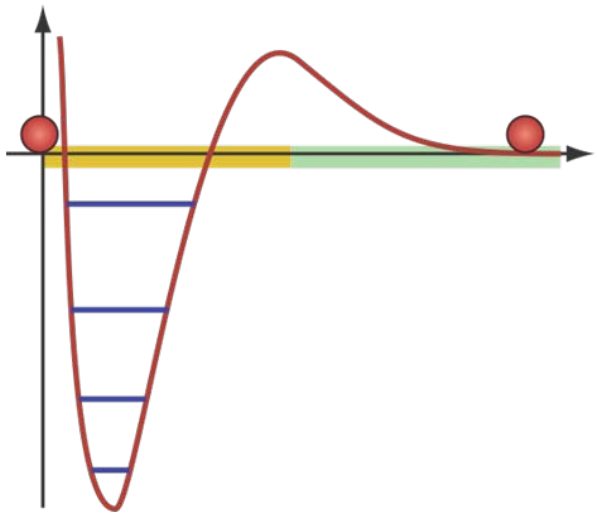
Elastic collisions

Effective potential

- low energy scattering dominated by the van der Waals part

- symmetric effective repulsion

$$V_{\text{eff}} \sim \frac{C_6}{r^6} \qquad C_6 = \frac{4C_6^{(0)} + 24C_6^{(2)}}{5}$$



- s-wave scattering length

$$a_s \approx 0.68 \left(\frac{C_6 m}{\hbar^2}\right)^{1/4}$$

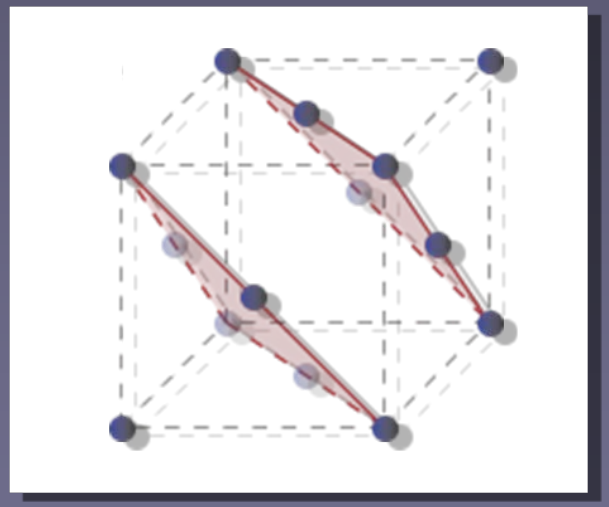
$$\approx 66\text{nm}$$

- large ratio between elastic and inelastic cross section

$$\frac{\sigma_{\text{el}}}{\sigma_{\text{ine}}} \sim 10^6 \qquad \text{at} \quad 1\,\text{mK}$$

route towards evaporative cooling of polar molecules

Cristalline phases



3D crystalline phases

Many-body Hamiltonian

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j) + \dots$$

angular dependence

$$V(\mathbf{r}) = C_6 f(\theta)/r^6$$

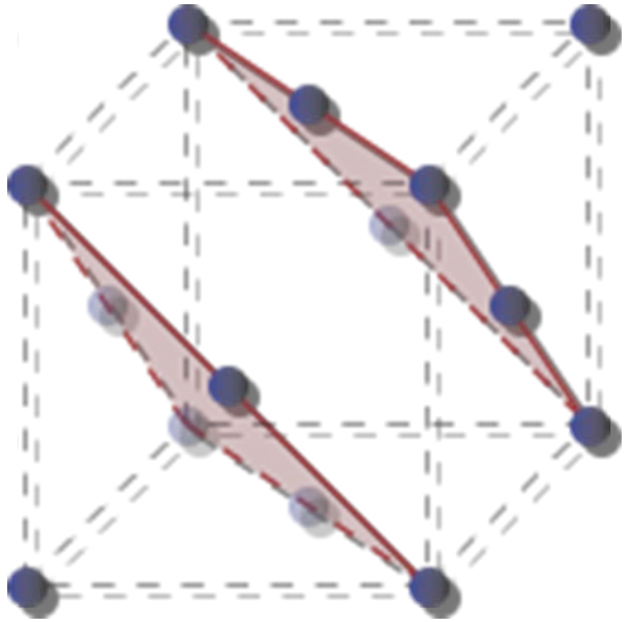
- dimensionless parameter

$$r_6 = \frac{E_{\rm int}}{E_{\rm kin}} = \frac{C_6 m}{\hbar^2} n^{4/3}$$

Cryalline phase

$r_6 \gg 1$

- closed packing for ellipsoid
- distored FCC lattice

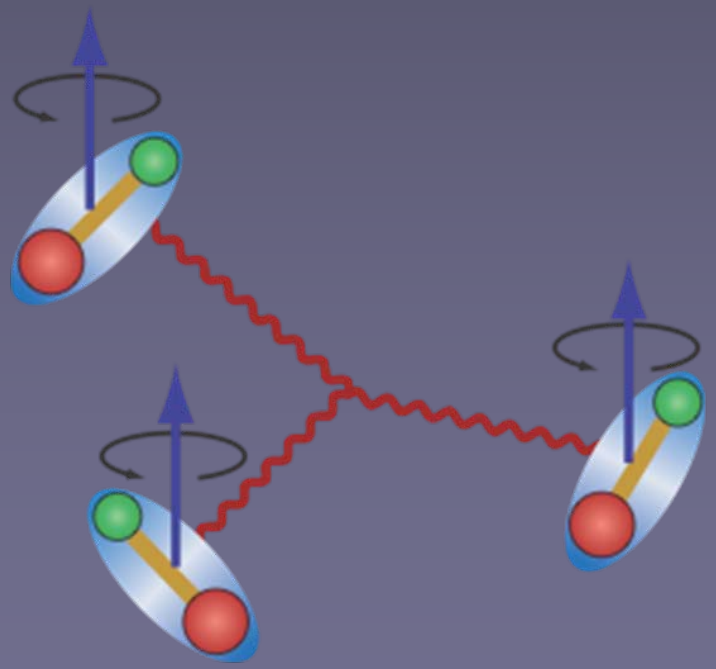


- realistic parameters for the lattice spacing

$$a \sim 100 - 300\text{nm}$$

- three-body interactions can

Three-body interactions



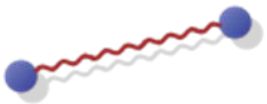
Three-body interactions

Many-body interaction potential

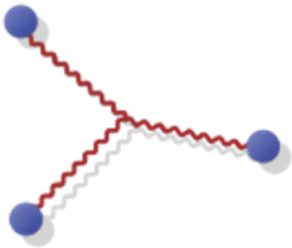
- Hamiltonians in condensed matter are effective Hamiltonians after integrating out high energy excitations

$$V_{\text{eff}}\left(\{\mathbf{r}_i\}\right) = \frac{1}{2}\sum_{i\neq j} V\left(\mathbf{r}_i - \mathbf{r}_j\right) + \frac{1}{6}\sum_{i\neq j\neq k} W\left(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k\right) + \dots$$

two-particle interaction



three-body interaction



Why is it interesting?

- novel tool for strongly correlated states

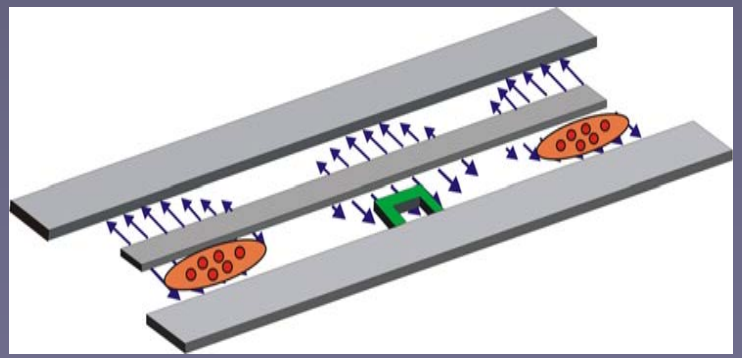
- Exotic phases
  - emergent symmetry
  - no spontaneous symmetry breaking: RVB, spin liquid, ...

- Topological phases
  - fractional quantum Hall states
  - (non)-abelian anyons
  - application in topological quantum computing

Do such phases exist in nature?

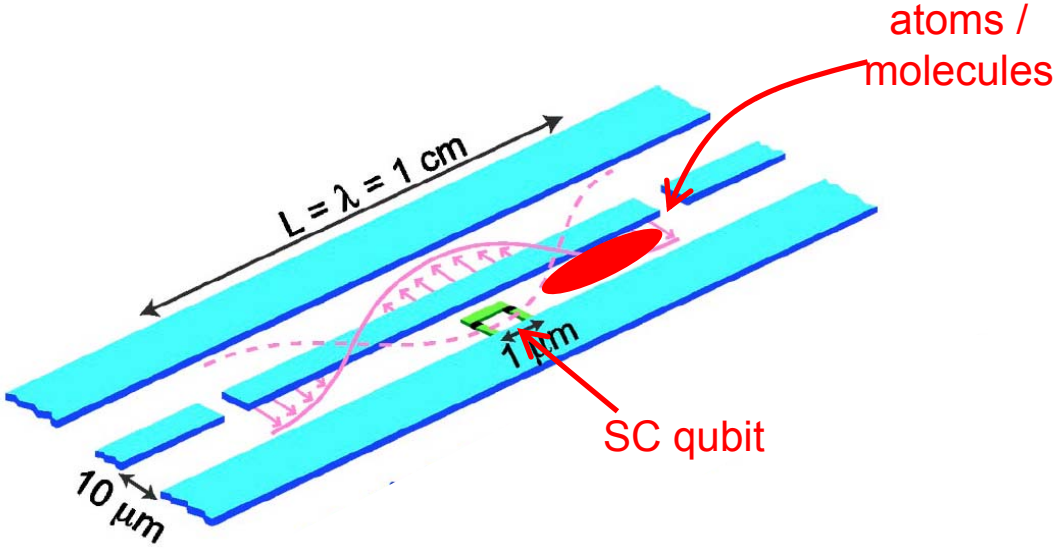
How often do they appear?

Circuit CQED and Molecular Quantum Memory

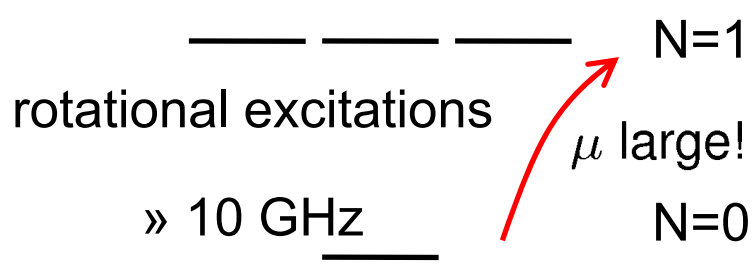


Molecular Quantum Memory

- **superconducting transmission line cavities**



- **rotational excitation of polar molecule(s)**



$$g \sim 2\pi \times 10 \text{ KHz } \sqrt{\#\text{molecules}}$$

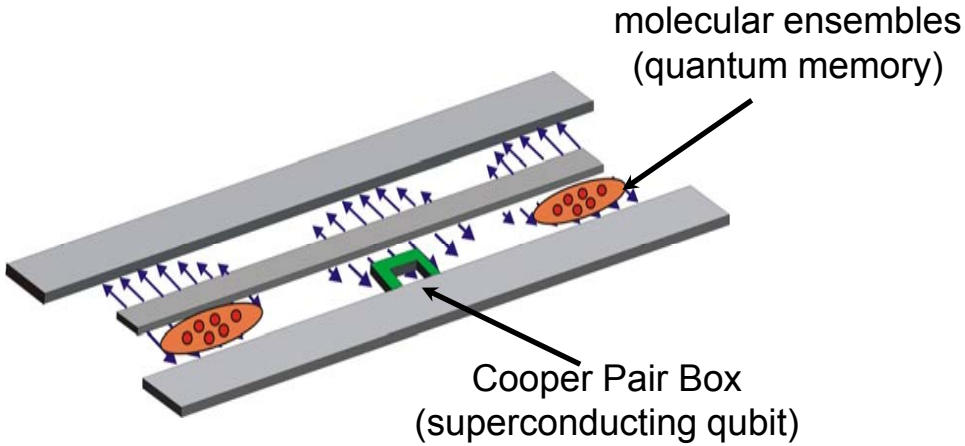
$$\sim 2\pi \times 1 \ldots 10\text{MHz}$$

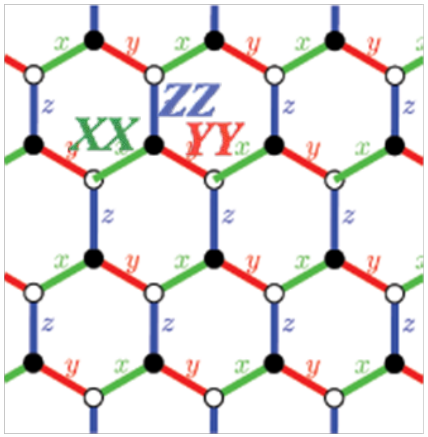
ensemble

Polar molecules

AMO- solid state interface

- solid state quantum processor
- molecular quantum memory
  (P. Rabl, D. DeMille, J. Doyle, M. Lukin,
  R. Schoelkopf and P. Zoller, PRL 2006)





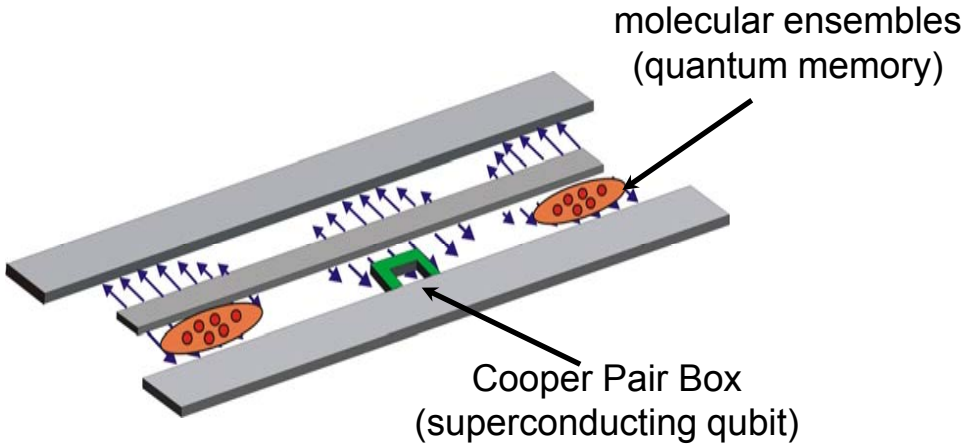
Spin toolbox

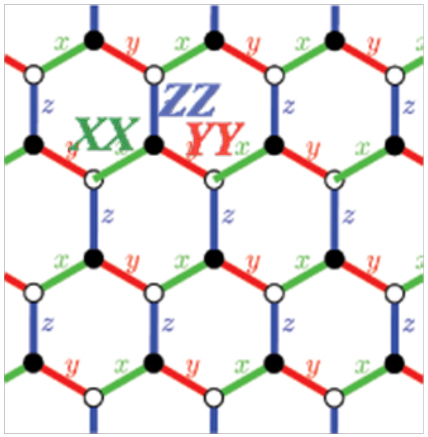
- polar molecules with spin
- realization of Kitaev model
  (A. Micheli, G. Brennen, P. Zoller,
  Nature Physics 2006)

Polar molecules

AMO- solid state interface

- solid state quantum processor
- molecular quantum memory
  (P. Rabl, D. DeMille, J. Doyle, M. Lukin,
  R. Schoelkopf and P. Zoller, PRL 2006)





Spin toolbox

- polar molecules with spin
- realization of Kitaev model
  (A. Micheli, G. Brennen, P. Zoller,
  Nature Physics 2006)