# Cold Atoms and Molecules:
# Condensed Matter Physics & Quantum Information

UNIVERSITY OF INNSBRUCK

- introduction / review
- topics in more detail: “quantum simulators”
  - dissipative Hubbard dynamics
  - engineering three-body Hubbard Hamiltonians

IQOQI
AUSTRIAN ACADEMY OF SCIENCES

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Collaborations:

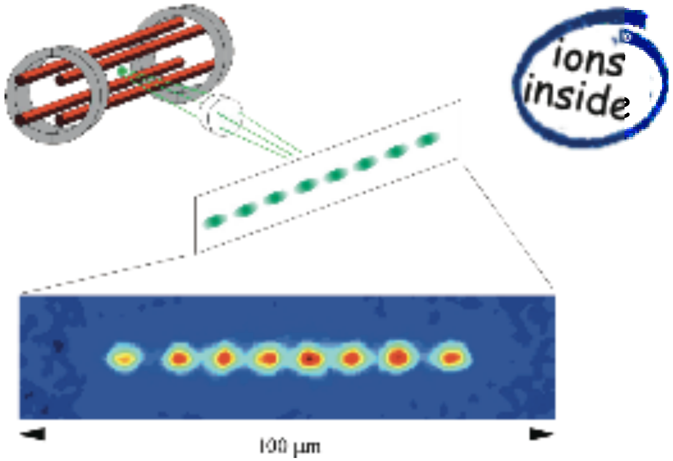
Harvard, Yale, Oxford

**SFB**
Coherent Control of Quantum Systems

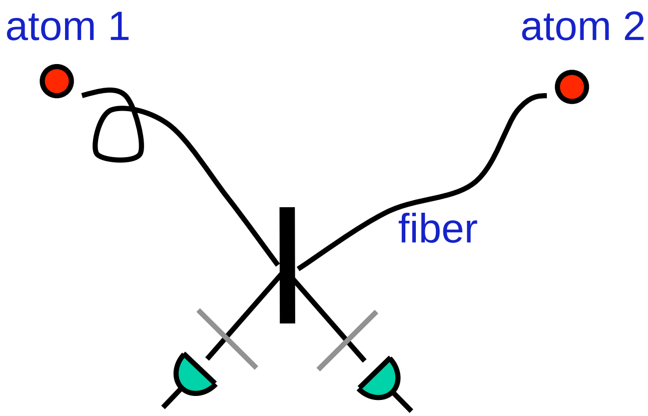
**€U networks**

## quantum optics

- trapped ions




- cavity QED: atom - photon interfaces

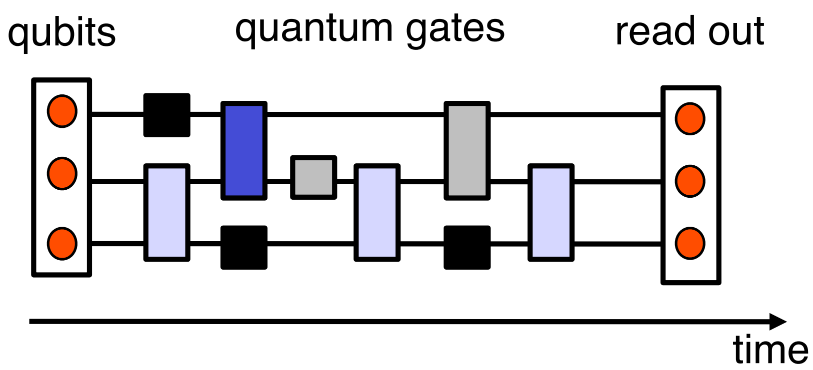



$$|\Psi\rangle \sim |01\rangle - |10\rangle$$

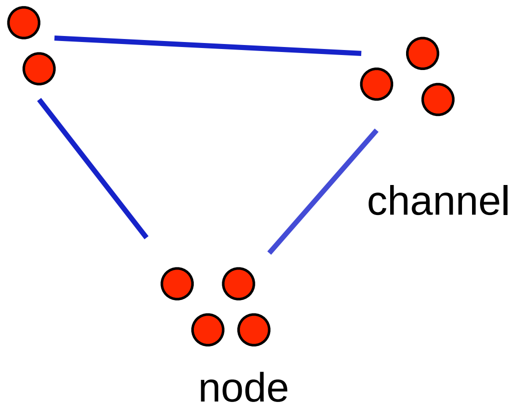
probabilistic generation of EPR state

## quantum info

- quantum computing: logic network



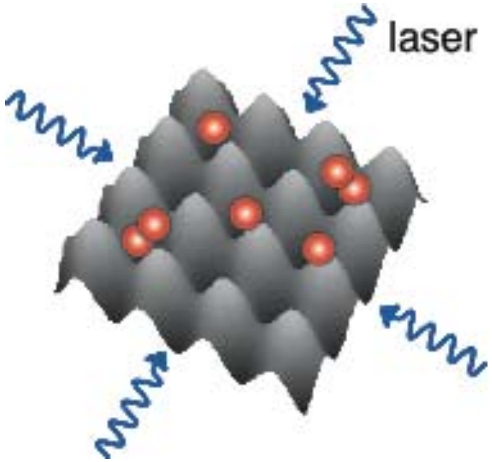

- building a network




quantum repeater

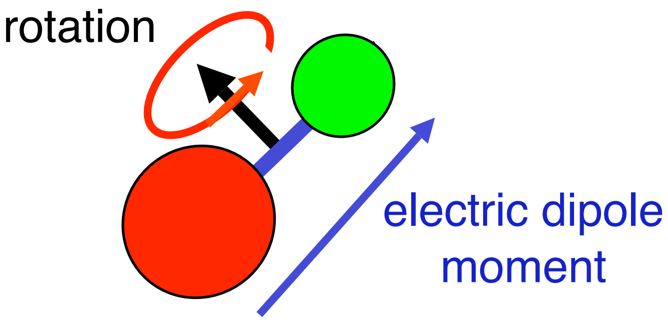
## quantum optics

- atoms in an optical lattices




- polar molecules

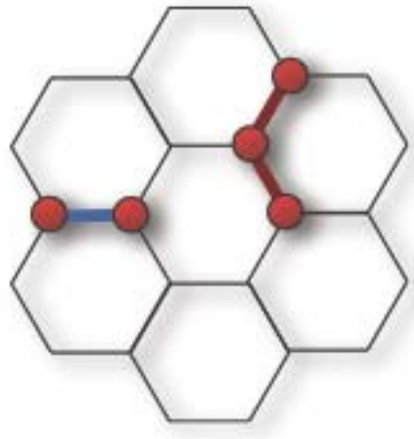
polar molecule in electronic
and vibrational ground state




*new system*

## cond mat & quantum info

- “quantum simulators” for cond mat models



2- & 3-body interactions

ring exchange

...

  - Hubbard & spin models
  - analog vs. digital quantum simulations

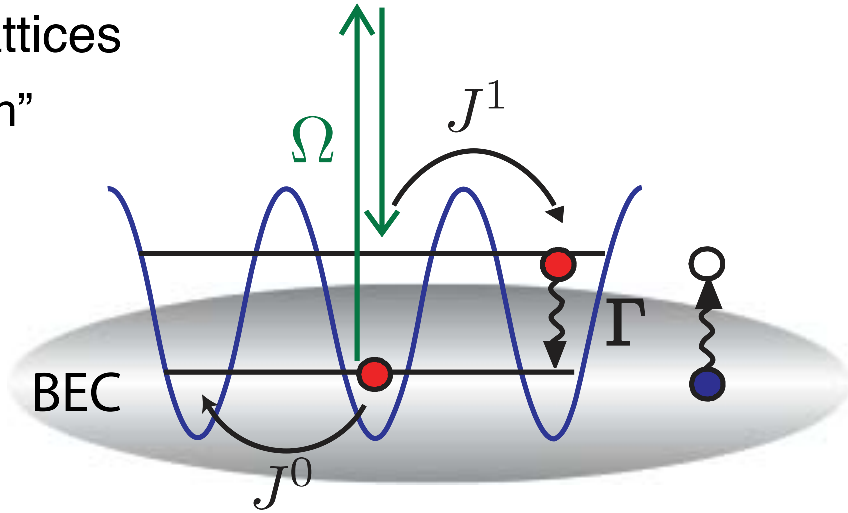
- measurement based quantum computing
- topological phases and qc (?)

(analog vs. digital quantum simulators)

# This talk ...

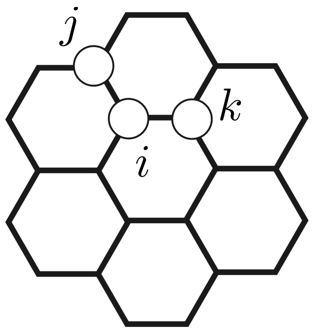
- Dissipative dynamics of atoms in optical lattices
  - immersion in a superfluid as a “phonon bath”
  - ... as  quantum optics problem
  - quantum reservoir engineering

  A. Griessner, A. J. Daley, S. R. Clark,
  D. Jaksch, PZ , PRL (2006); NJP (2007)



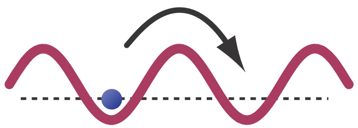

- Hubbard, spin models (with polar molecules)
  - short review of ideas and models
  - three-body interactions

$$H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{1}{2} \sum_{i \neq j} \cancel{U_{ij}} n_i n_j + \frac{1}{6!} \sum_{i \neq j \neq k} W_{ijk} n_i n_j n_k .$$

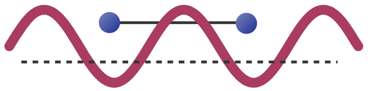



compare: string net
Fidkowski et al.,
cond-mat/0610583

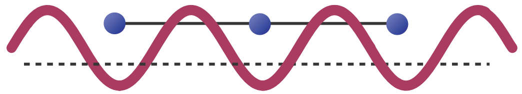
hopping



*tunable* two-body
interaction



*strong repulsive* off-site
three-body interaction



H.P. Büchler, A. Micheli, PZ, preprint

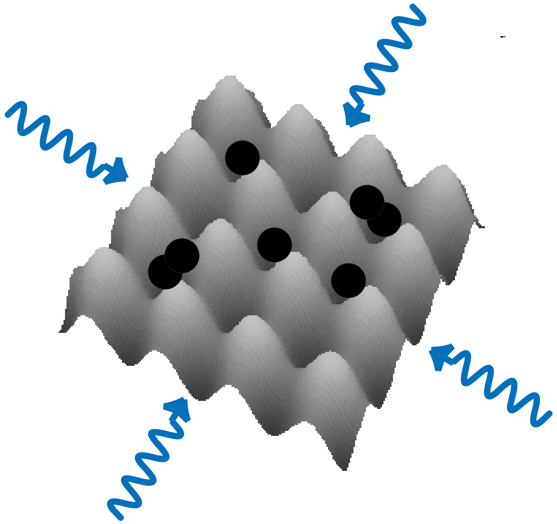
## Dissipative dynamics of cold atoms in optical lattices

- quantum optics with cold atoms

Jaksch et al. PRL 1998

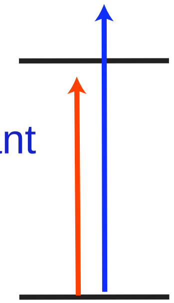
# Cold atoms in optical lattices:
# 1. Coherent Hubbard dynamics

- Loading bosonic or fermionic atoms into optical lattices
- Atomic Hubbard models with controllable parameters
  - bose / fermi in 1,2&3D
  - spin models
  - "AMO Hubbard toolbox"

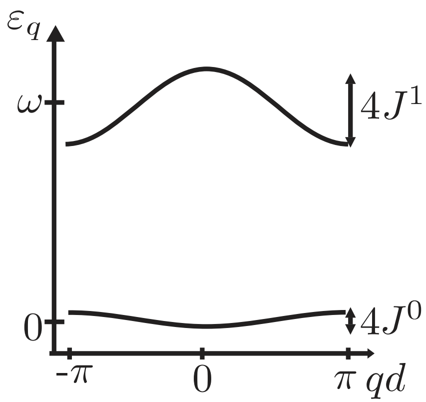


optical lattice as array of microtraps

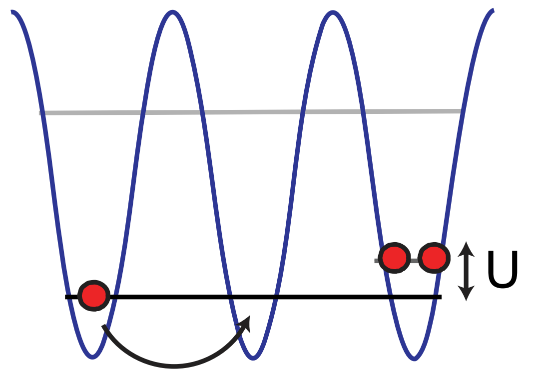
nonresonant laser



AC Stark shift




band structure (1D)




onsite interaction

$J$ tunneling

$$\hat{H} = -\sum_{\alpha\neq\beta} J_{\alpha\beta}\hat{a}^\dagger_\alpha a_\beta + \frac{1}{2}U\sum_\alpha \hat{a}^\dagger_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha \hat{a}_\alpha$$

single band Hubbard model

kinetic energy: hopping

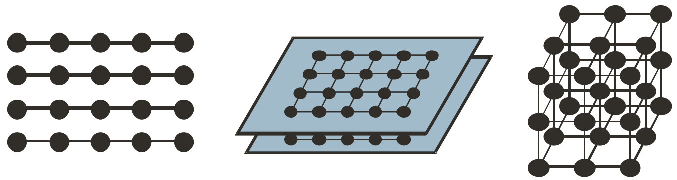
interaction: onsite repulsion

"(analog) quantum simulators"

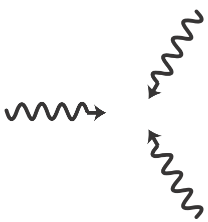
D. Jaksch & PZ,
Annals of Physics 2005

# AMO Hubbard toolbox

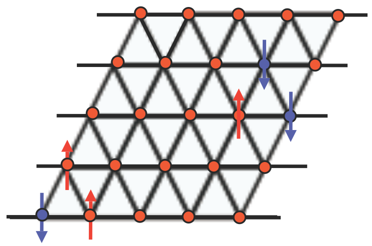
- time dependence
- 1D, 2D & 3D



- various lattice configurations

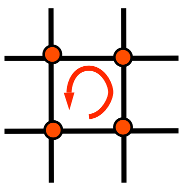


laser



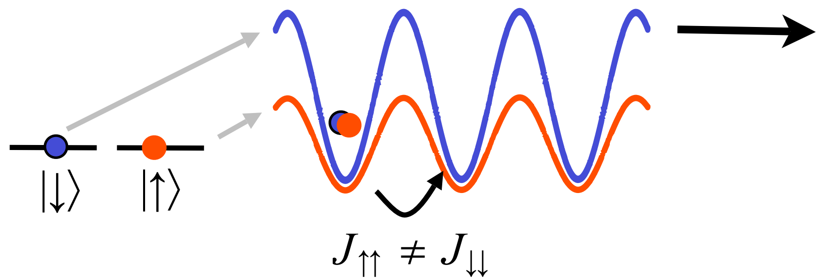
triangular lattice

- create effective magnetic fields



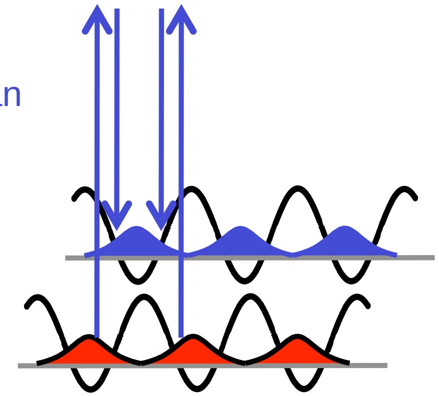
$$J_{\alpha\beta} \longrightarrow J_{\alpha\beta}\, e^{ie\int_\alpha^\beta \vec{A}\cdot d\vec{l}}$$

- spin-dependent lattices



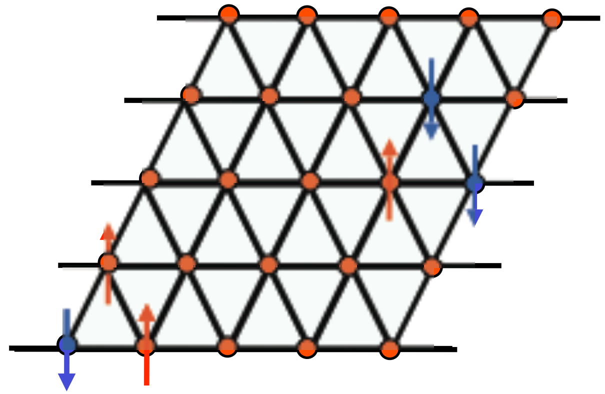

- laser induced hoppings

Raman

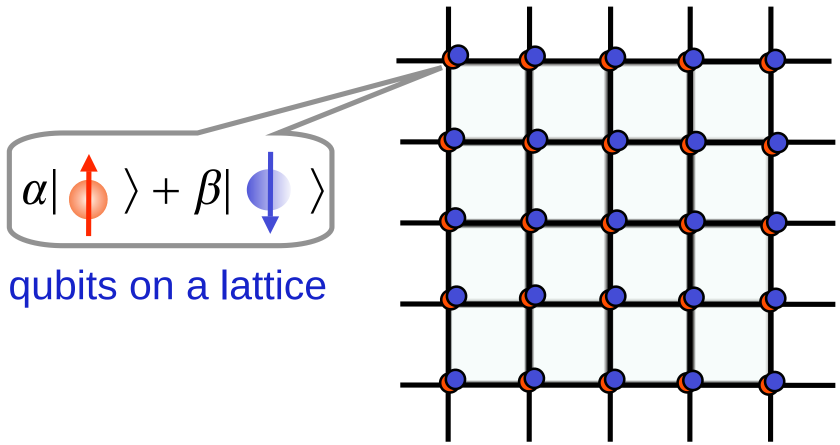


# Why? … condensed matter physics & quantum information

- condensed matter systems
  - strongly correlated systems
  - time dependence, e.g quantum phase transitions
  - ...
  - exotic quantum phases(?)



- quantum information
  - new quantum computing scenarios, e.g. one way quantum computing




qubits on a lattice

entangling qubits via "Ising" (cluster state)

analog & digital
quantum simulators

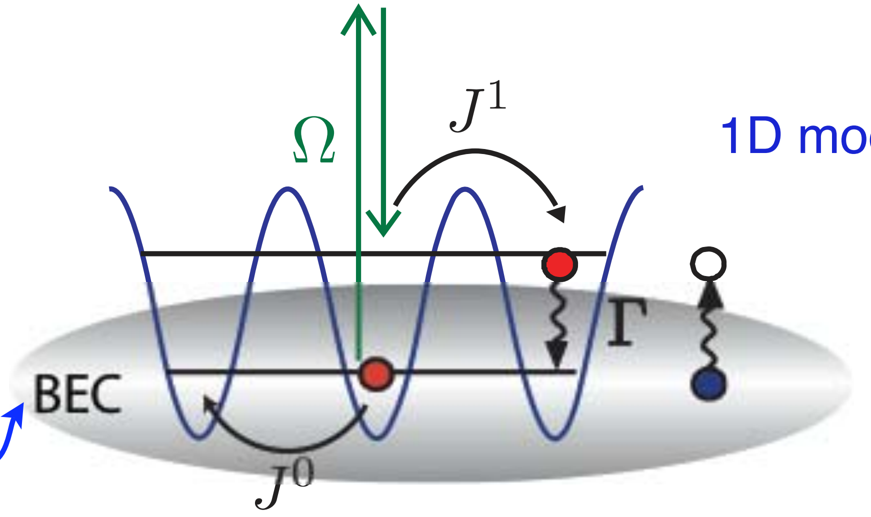
- experiments [Bloch et al. 2001, Esslinger, Porto, Grimm & Denschlag …]

A. Griessner et al. PRL 2006; NJP 2007

# 2. Dissipative Hubbard dynamics

- BEC as a “phonon reservoir”
  - quantum reservoir engineering

1D model




does not see the optical lattice

- master equation:

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \mathscr{L}\hat{\rho}$$

- validity (as in quantum optics)
  - ✓ interband transitions
  - ✓ RWA + Born + Markov

- coherent Hubbard dynamics

$$H = \ldots$$

✓ two band Hubbard model (1D)
✓ + Raman coupling

- dissipative dynamics

$$\mathscr{L}\rho = \sum_k \frac{\Gamma_k}{2}\left(2c_k\hat{\rho}c_k^\dagger - c_k^\dagger c_k\hat{\rho} - \hat{\rho}c_k^\dagger c_k\right)$$

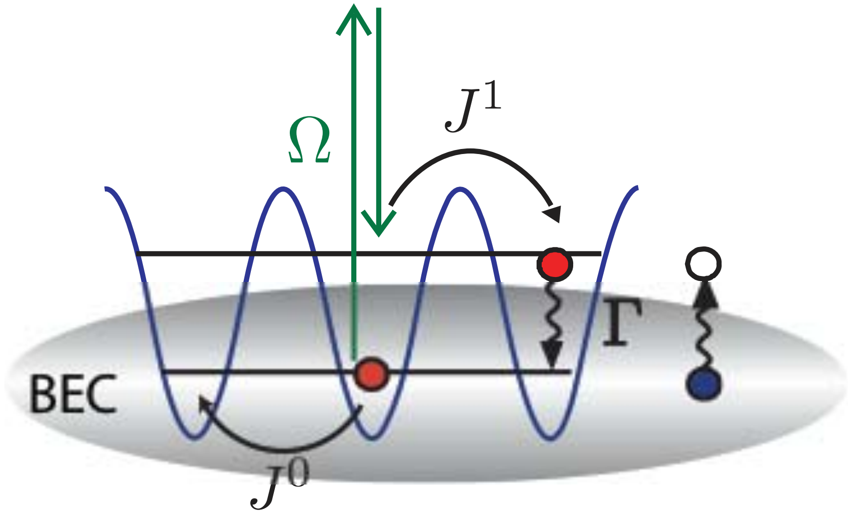
quantum jump operator

competing dynamics

A. Griessner et al. PRL 2006; NJP 2007

# 2. Dissipative Hubbard dynamics

- BEC as a "phonon reservoir"
  - quantum reservoir engineering




- master equation:

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \mathscr{L}\hat{\rho}$$

---

as opposed to ...

- Caldeira-Leggett
  - linear system-bath couplings, ohmic / superohmic
  - quantum phase transitions in Josepshon Junction arrays
- polarons
- phonon mediated interactions

# Why (controlled dissipation)?

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \mathscr{L}\hat{\rho}$$

competing dynamics

- why? engineering reservoirs for ...
  - dissipative quantum phase transitions / crossover
  - ...
  - applications: cooling etc.

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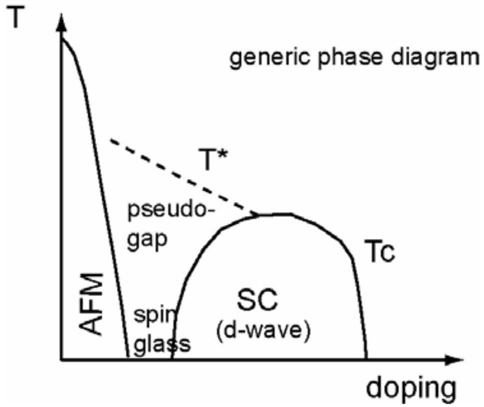
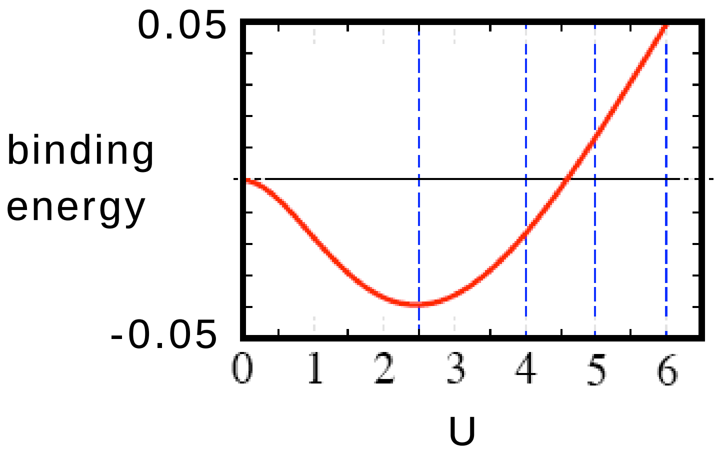
- Anderson (1987): ground state = resonating valence bond state

high-Tc superconductors




binding energy 4% of width of Bloch band

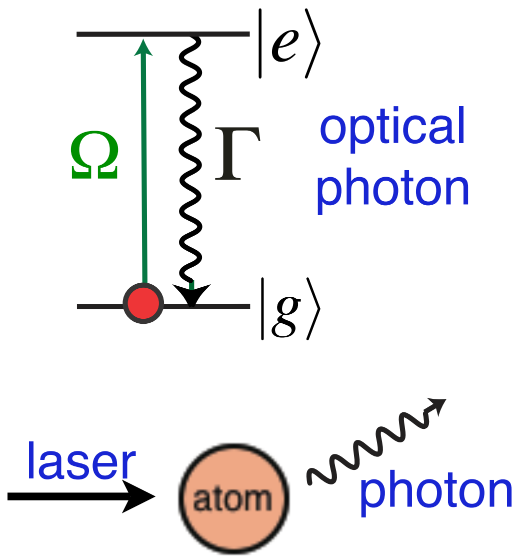
(units of hopping t)

minimal model: two-dimensional one-band Hubbard model

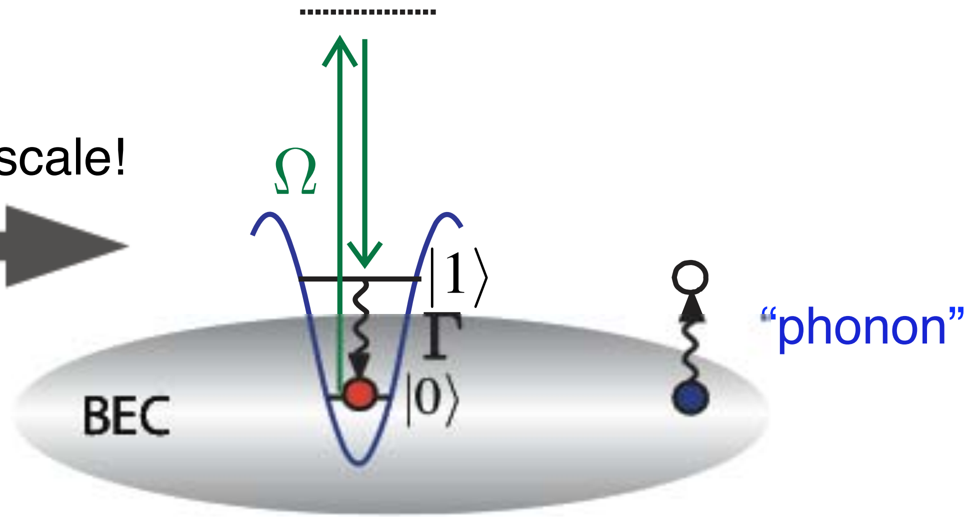
$$\hat{H} = -t \sum_{<ij>,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i$$

# “think quantum optics”

- driven two-level atom + spontaneous emission
- trapped atom in a BEC reservoir




energy scale!




laser assisted atom + BEC collision

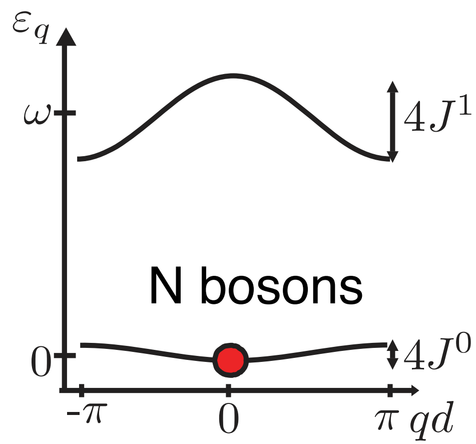
- reservoir: vacuum modes of the radiation field (T=0)
- reservoir: Bogoliubov excitations of the BEC (@ temperature T)
- optical pumping, laser cooling, ...
  - purification of electronic, and motional states

$$\rho_a \otimes |\mathrm{vac}\rangle\langle\mathrm{vac}| \rightarrow |\psi_a\rangle\langle\psi_a| \otimes \rho'$$

?

# Models ...

- **Model A: Dark state cooling in a Bloch band** (“dark state laser cooling”)
  - single atom
  - N non-interacting atoms + adiabiatic turn on off interactions




- **Model B: Master equations N interacting atoms**

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \mathscr{L}\hat{\rho}$$

Hubbardology

Hubbard dynamics
(superfluid / Mott)

quantum reservoir engineering

coupling to a local current drives system
into N-body dark state

$$|\psi_{\mathrm{BEC}}\rangle = \frac{1}{\sqrt{N!}}\left(\sum_i a_i^\dagger\right)^N |\mathrm{vac}\rangle$$

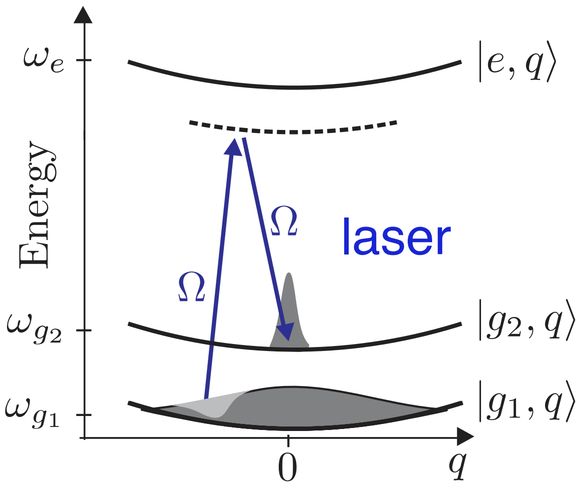
competing dynamics

work in progress

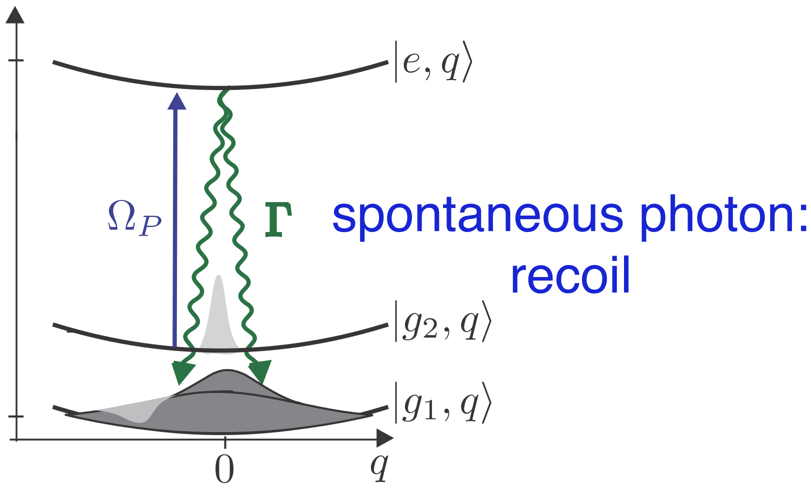
# Subrecoil ("dark state") laser cooling

**Raman subrecoil cooling (Kasevich and Chu)** (see also: VSCPT Cohen et al.)

step 1: excitation & filtering




step 2: diffusion

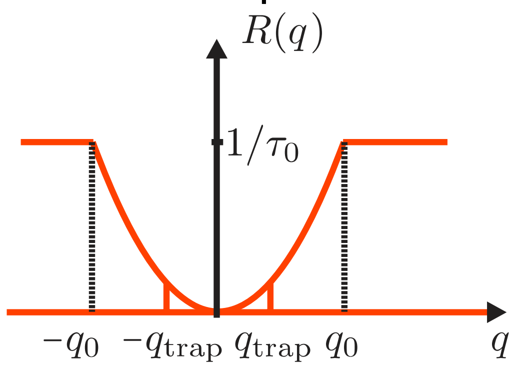



- "dark state" laser cooling: accumulate atoms near q≈0

# Levy statistics approach (Cohen-Tannoudji et al.)

- excitation profile and trapping region

excitation profile:



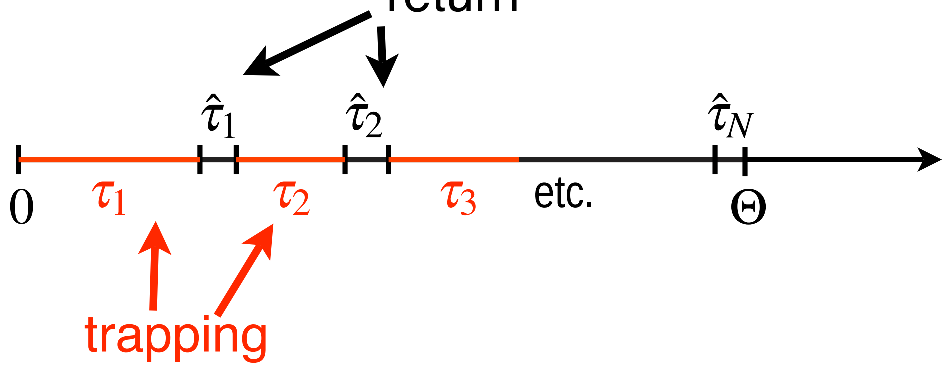

trapping region

$$R(q) \sim |q|^{\lambda}$$

$\lambda = 2$ square pule

$\lambda = 4$ Blackman pulse

- time evolution




✓ trapping times

$$P(\tau) \sim \tau^{-(1+1/\lambda)}$$

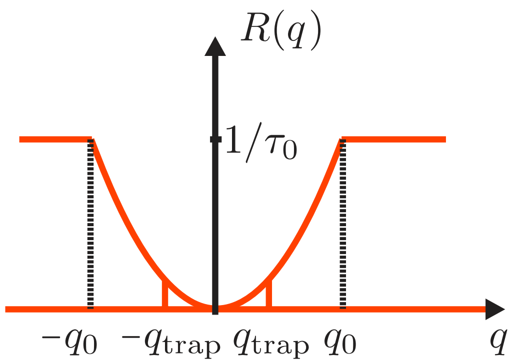
$$\langle\tau\rangle \to \infty \quad (\lambda > 1)$$

$$T(N) = \sum_{i=1}^{N} \tau_i \sim N^{\lambda}$$

generalized central limit theorem

✓ return times

$$\hat{T}(N) = \sum_{i=1}^{N} \hat{\tau}_i \sim N\langle\tau\rangle$$




trapping region

$$R(q) \sim |q|^{\lambda}$$

iff $\lambda > 1$, then all atoms for $\Theta = T(N) + \hat{T}(N) \to \infty$ in cooling region

temperature $$\frac{1}{2}k_B T = \frac{\delta q^2}{2m} \sim \Theta^{-2/\lambda}$$

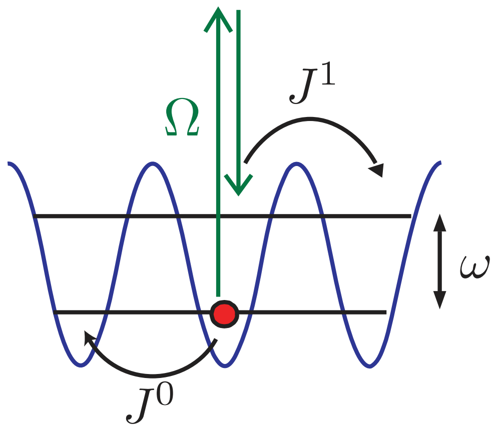
$$n_0(\Theta) \sim \Theta^{1/\lambda}$$

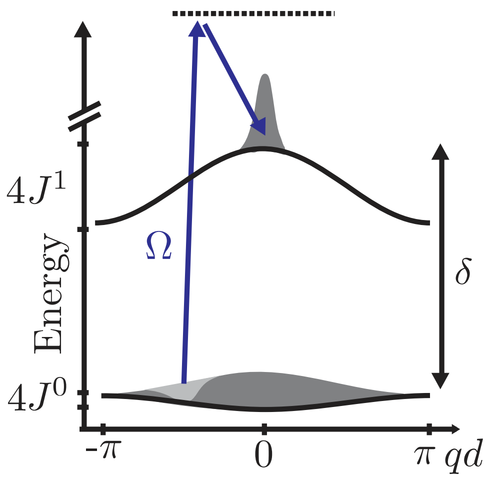
time

A. Griessner et al. PRL 2006;
NJP 2007

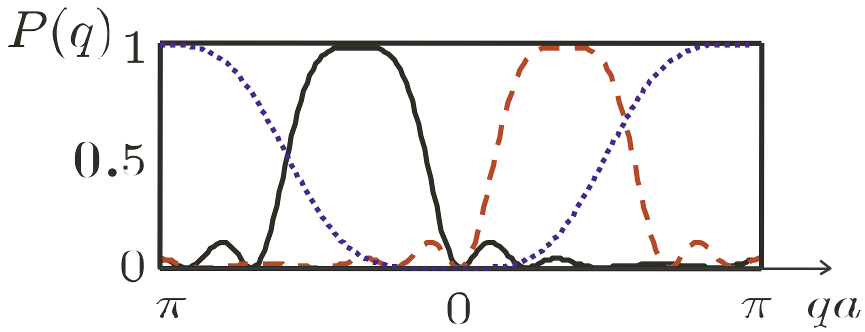
# Raman cooling within a Bloch band: qualitative

- step 1: (coherent) quasimomentum selective excitation




Laser: square pulse sequence



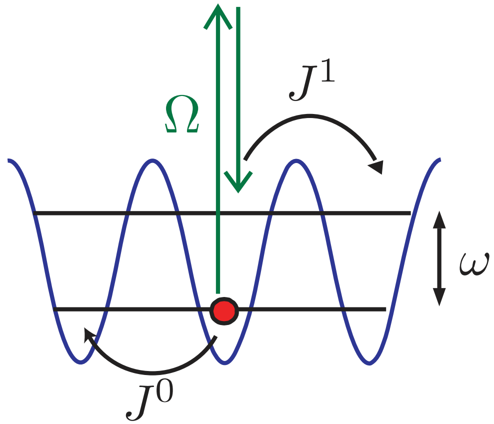

$$P(q) = \frac{\Omega^2}{(\delta_{q+\delta q}^2 + \Omega^2)} \sin^2\left(\sqrt{\delta_{q+\delta q}^2 + \Omega^2}\,\tau/2\right)$$

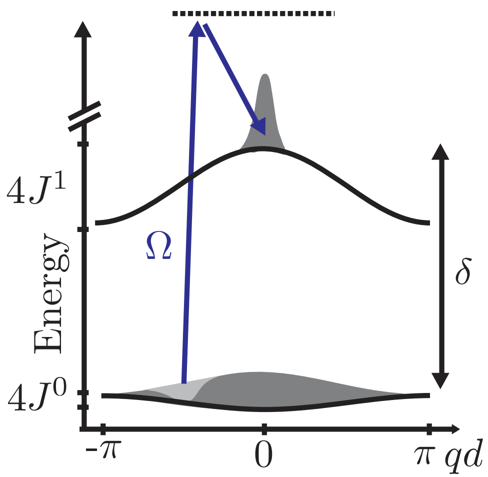
- requirements: $\Omega \ll 8|J^1|$
- Note: relevant energy scale given by $|J^1|$

A. Griessner et al. PRL 2006; NJP 2007

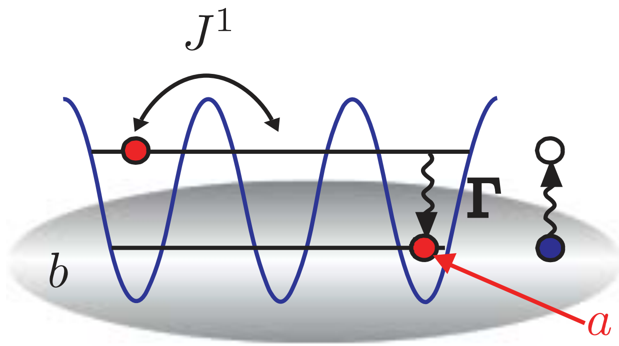
# Raman cooling within a Bloch band: qualitative

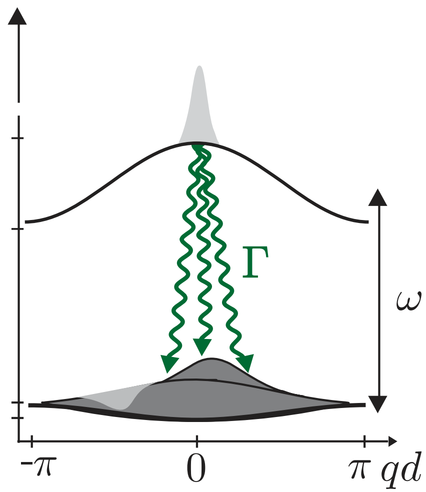
- step 1: (coherent) quasimomentum selective excitation



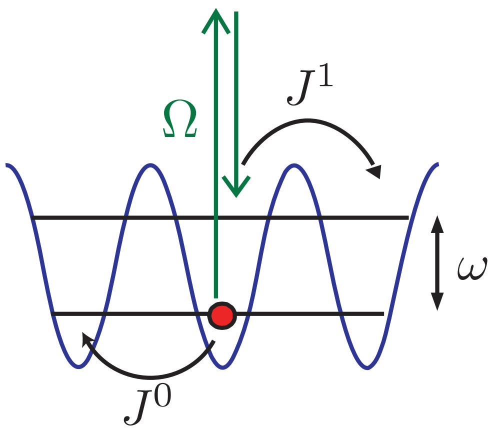

- step 2: (dissipative) decay to ground band

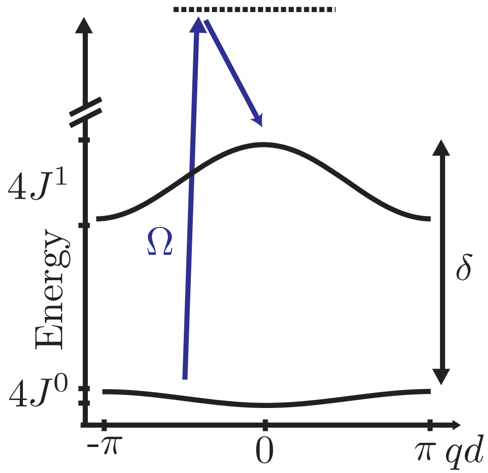


# Model: 1. Coherent dynamics

- 1D lattice




Bloch bands

- Hamiltonian

$$\hat{H}_0 = \sum_{q,\alpha} \varepsilon_q^\alpha \left(\hat{A}_q^\alpha\right)^\dagger \hat{A}_q^\alpha + (\omega - \delta) \sum_q \left(\hat{A}_q^1\right)^\dagger \hat{A}_q^1 + \frac{\Omega}{2} \sum_q \left[\left(\hat{A}_q^1\right)^\dagger \hat{A}_{q-\delta q}^0 + \text{h.c.}\right]$$

Rabi freq.

$$\varepsilon_q^\alpha = -2J^\alpha \cos(qd)$$

Bloch band

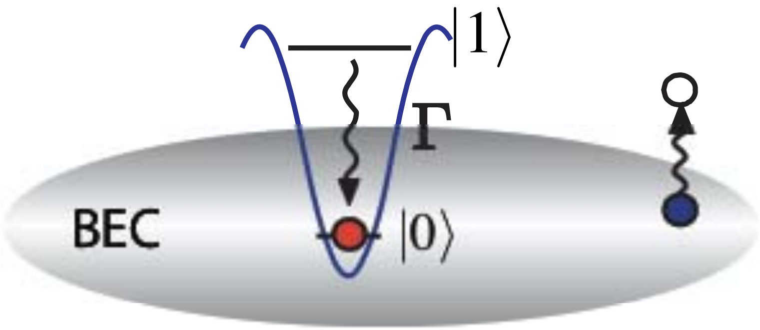
$$\hat{H}_I = \frac{1}{2M} \sum_{q_1,q_2,q_3,\alpha} U^{\alpha\beta} \left(\hat{A}_{q_1}^\beta\right)^\dagger \left(\hat{A}_{q_2}^\alpha\right)^\dagger \hat{A}_{q_3}^\alpha \hat{A}_{q_1+q_2-q_3}^\beta$$

tune via scattering length

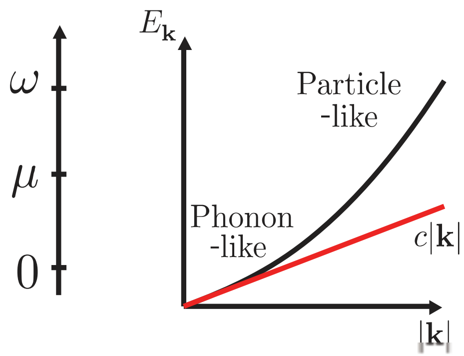
collisional interactions

validity: $J^\alpha, U^{\alpha,\beta'}, \Omega \ll \omega,\ \omega \ll \omega_\perp$

# Model: 2. “Spontaneous Emission”




spectrum of
Bogoliubov excitations




$$\varepsilon_k = [c^2(\hbar k)^2 + (\hbar k)^4/(2m_b)^2]^{1/2}$$

- BEC reservoir

$$\hat{H}_{\mathrm{BEC}} = E_0 + \sum_{\mathbf{k}\neq 0} \varepsilon(\mathbf{k})\, \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}}$$

$$\hat{\psi}_b = \sqrt{\rho_0} + \delta\hat{\psi}_b$$

$$\delta\hat{\psi}_b = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \left( u_{\mathbf{k}} \hat{b}_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{r}} + v_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{r}} \right)$$

Bogoliubov

- interaction: interband 0 - 1

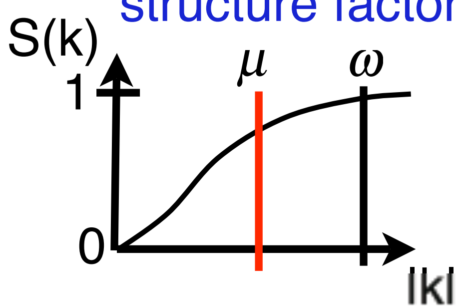
$$\hat{H}_{\mathrm{int}} = g_{ab} \int \hat{\psi}^\dagger_a(\mathbf{r})\, \hat{\psi}_a(\mathbf{r})\, \hat{\psi}^\dagger_b(\mathbf{r})\, \hat{\psi}_b(\mathbf{r}) \mathrm{d}^3\mathbf{r}$$

$$\sim g_{ab} \sum_{\mathbf{k}} S(\mathbf{k},\omega)^{1/2} \langle w_1|\mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{r}}|w_0\rangle \hat{b}_{\mathbf{k}} |1\rangle\langle 0| + \mathrm{h.c.}$$

$\approx 1$

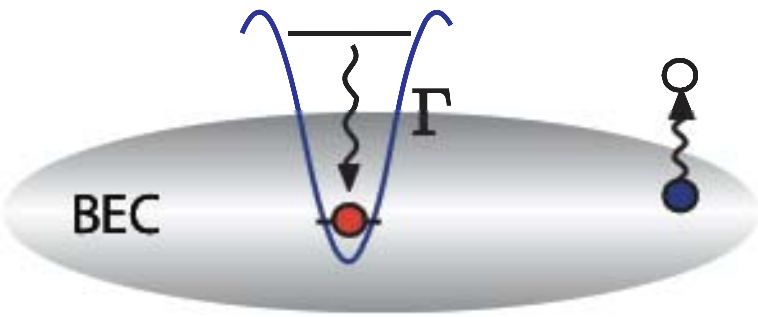
“spontaneous emission”

structure factor

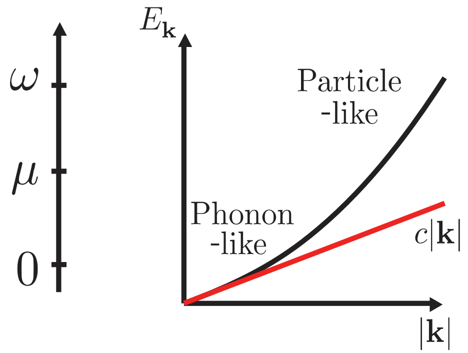



$$S(\mathbf{k}) = (u_{\mathbf{k}} + v_{\mathbf{k}})^2 = \frac{|\mathbf{k}|^2}{2m_b E_{\mathbf{k}}}$$

# “Spontaneous Emission”




spectrum of
Bogoliubov excitations




- interband transitions spontaneous emission rate
  - typical numbers

$$\Gamma = 2\pi \times 1.1 \text{ KHz}$$

weak coupling

$$a_s = 100 a_0$$ scattering length

$$\rho_0 = 5 \times 10^{14} \text{cm}^{-3}$$ density

$$\omega = 2\pi \times 100 \text{ KHz}$$ trap frequency

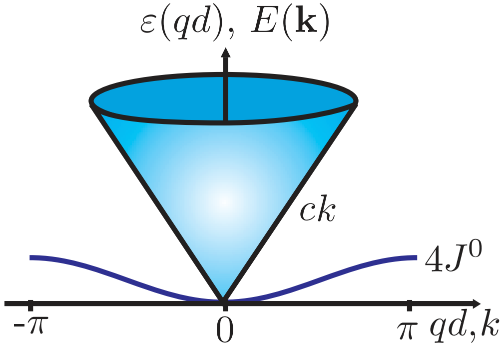
  - tunability

$$\Gamma \sim \rho_0 a_s^2 \sqrt{\omega}$$

scattering length:
magnetic or optical Feshbach resonance
density

- interaction: intraband ...

$$\begin{aligned}\varepsilon^0_{q\approx 0} &= \varepsilon^0_{q'} + c|\mathbf{k}| \\ q &= q' + k\end{aligned}$$




forbidden if $J^0 < \dfrac{\sqrt{\mu\omega_R m_a/(2m_b)}}{\pi}$

✓ no heating / cooling due to intraband transitions

✓ we ignore intraband processes in the following

✓ Rem.: validity of master equation ...

We can cool to temperatures lower than the BEC

# Master equation

- ... in analogy with spontaneous emission ($k_B T \ll \hbar\omega$, i.e. $T = 0$)

$$\mathscr{L}\hat{\rho} = \sum_k \frac{\Gamma_k}{2}\left(2c_k\hat{\rho}c_k^\dagger - c_k^\dagger c_k\hat{\rho} - \hat{\rho}c_k^\dagger c_k\right)$$

1D momentum
along lattice axis

$$|k| \leq k_{\max} = \sqrt{2m_b\omega}$$

energy conservation

quantum jump
operator

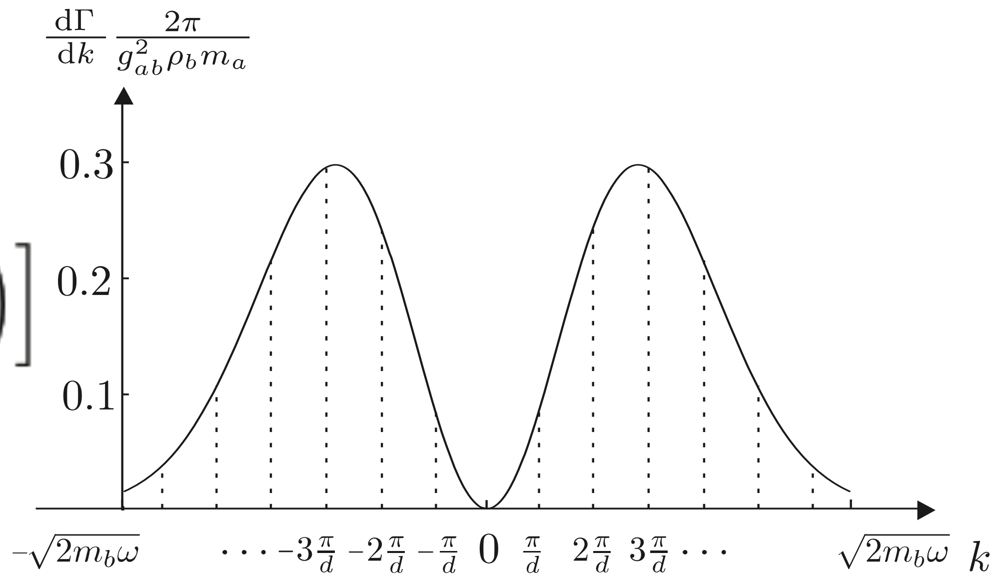
$$c_k \equiv \sum_j (\hat{a}_j^0)^\dagger(\hat{a}_j^1)\mathrm{e}^{-ikx_j} = \sum_q (\hat{A}^0_{q-k})^\dagger \hat{A}^1_q$$

modulo first Brillouin zone

- spontaneous emission rate $\Gamma = \sum_k \Gamma_k$

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}k} \hat{=} \frac{L}{2\pi}\Gamma_k = \frac{g_{ab}^2\rho_b m_a a_0^2 k^2}{4\pi}\mathrm{e}^{-a_0^2k^2/2}$$

$$\Gamma = \frac{g_{ab}^2\rho_b m_b}{2\pi a_0}\left[\sqrt{2\frac{m_b}{m_a}}\mathrm{e}^{-\frac{m_b}{m_a}} - \sqrt{\frac{\pi}{2}}\mathrm{erf}\left(\sqrt{\frac{m_b}{m_a}}\right)\right]$$



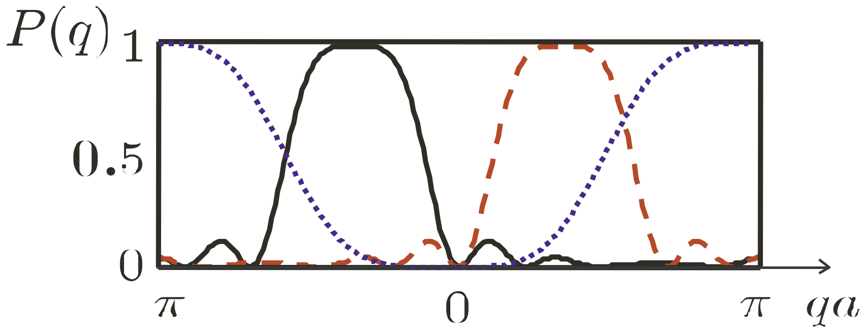

(1) $k_{\max} \gg \pi/d$, no superradiance

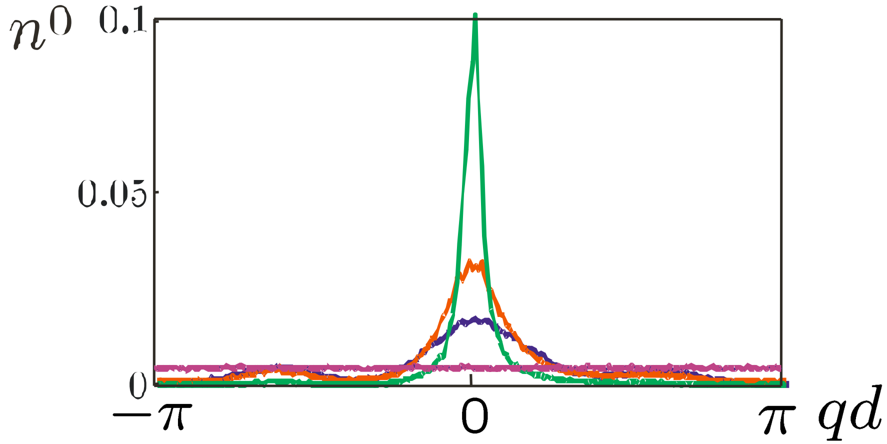
(2) $k_{\max} < \pi/d$. [superradiance]

# Results: single atoms

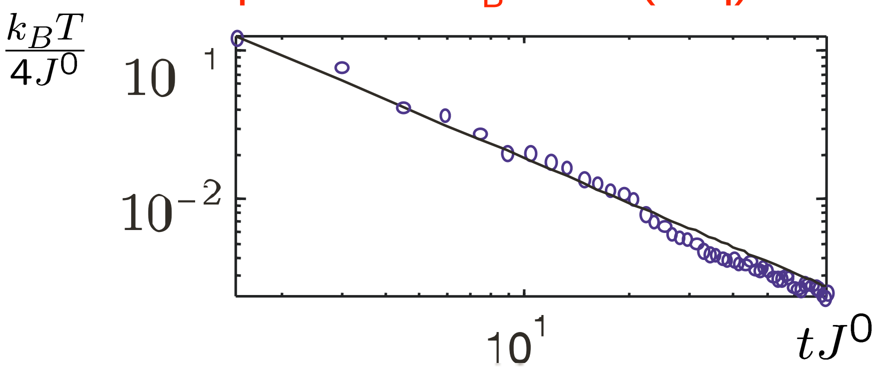
- Ground state q=0 momentum peak $4J^0 \ll k_B T \ll \omega$.
- Quantum trajectory simulation of the master equation

Laser: square pulse sequence

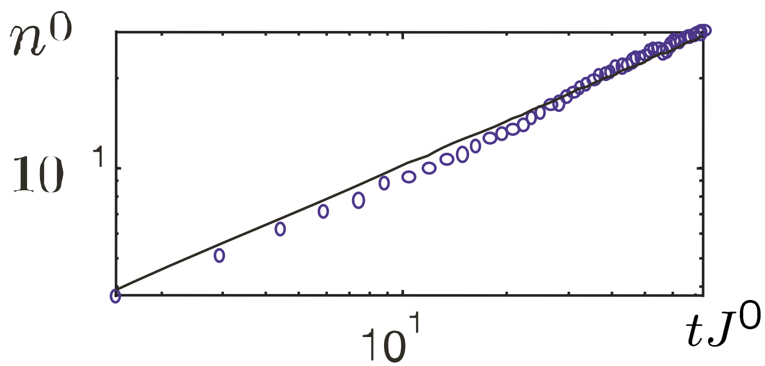



Temperature: $k_B T = 2J^0(\Delta q)^2$




Dark state occupation: $n^0(q=0)$




- Typical temperatures $k_B T/4J^0 \sim 2 \times 10^{-3}$ in $t_f J^0 \sim 50$
- Analysis in terms of Levy flights

# Many (non-interacting) bosons

- Assume: we can switch off interaction between bosons $a_{aa} \to 0$ with Feshbach resonance; independent bosons
- Ground state cooling: $q = 0$ peak in momentum distribution
- Numerical analysis: Quantum Boltzmann master equation

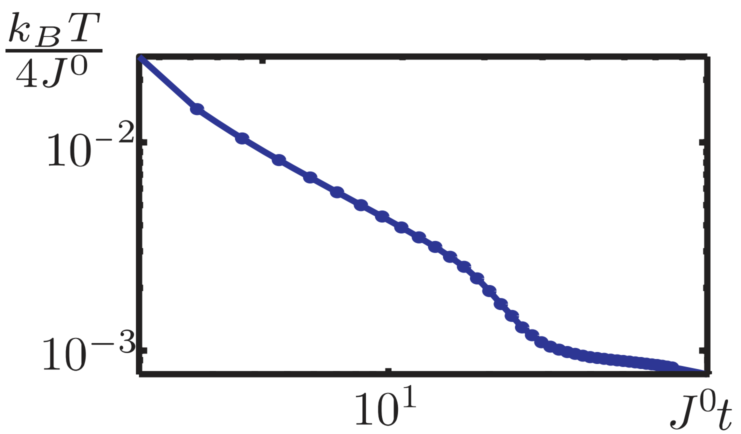
$$\dot{w}_{\mathbf{m}} = \sum_{k,q} \Gamma_k \left[ \mathrm{m}^0_{q-k}(1 \pm \mathrm{m}^1_q) w_{\mathbf{m}'} - \mathrm{m}^1_q (1 \pm \mathrm{m}^0_{q-k}) w_{\mathbf{m}} \right]$$

occupation of momentum state $q$ in Bloch band

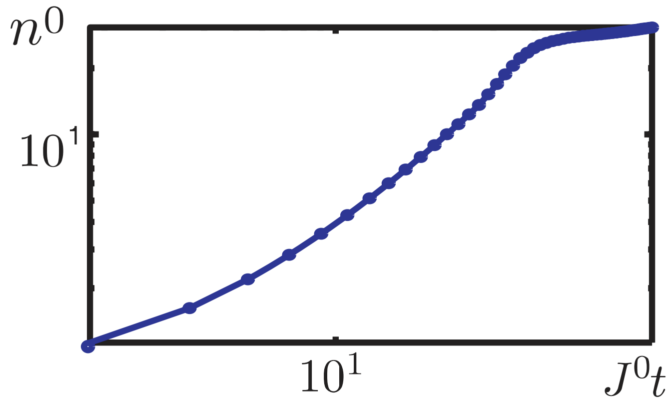
We failed to apply DMRG type ideas because our temperatures are too low ☹

QBME is a rate equation for $w_{\mathbf{m}} \equiv \langle \mathbf{m} | \rho | \mathbf{m} \rangle$, i.e. classical configurations $w_{\mathbf{m}}$ of atoms occupying momentum states $\mathbf{m} = [\{m^0_q\}_q, \{m^1_q\}_q]$ in the two Bloch bands.

Temperature:



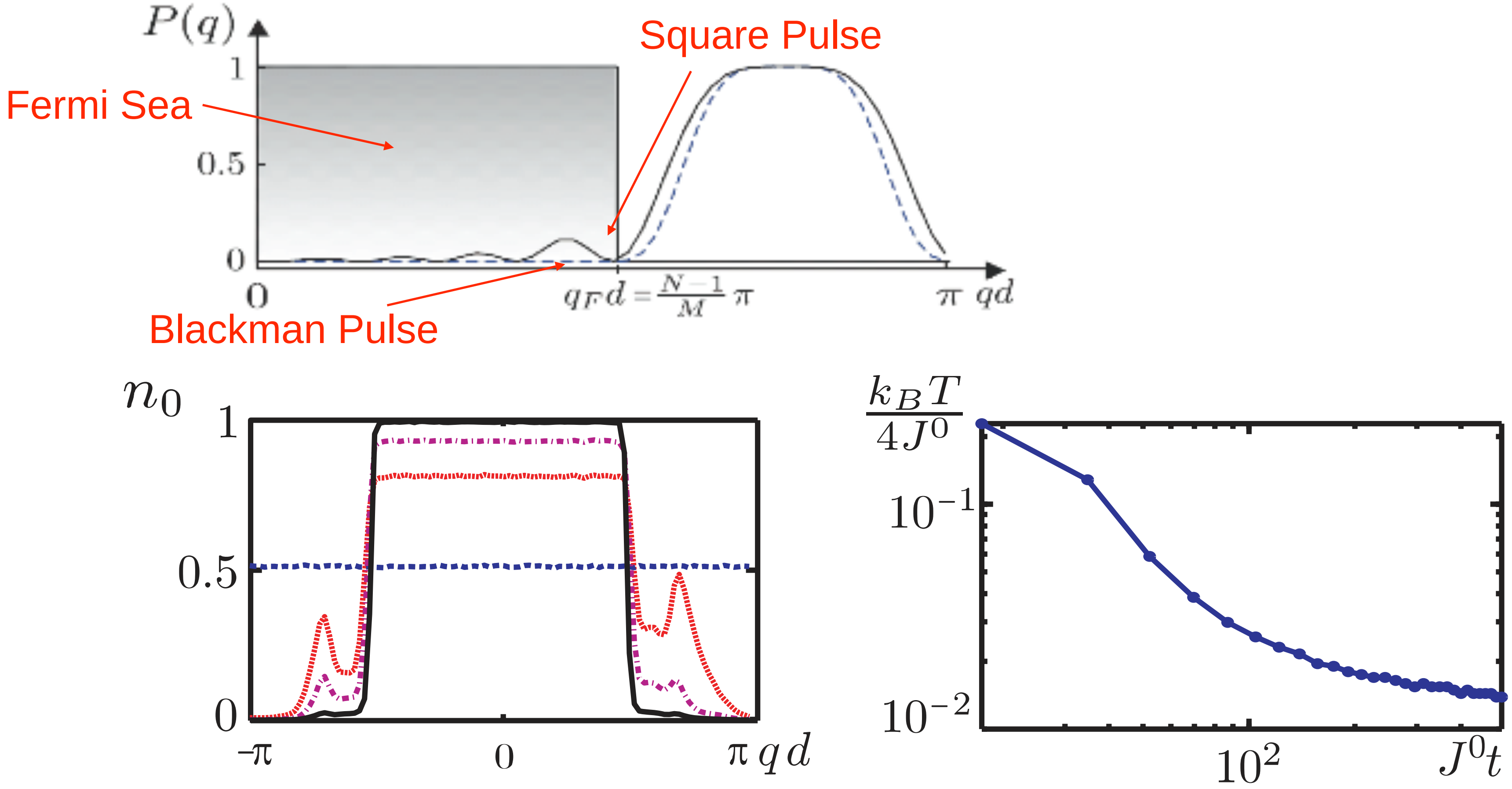

Dark state occupation: $n^0(|qd|<0.06)$




- Bosonic enhancement of cooling

# Many fermions

- Many spin-polarized (non-interacting) fermions
- Ground state: filled Fermi sea




- Typical temperatures $k_B T/4J^0 \sim 10^{-2}$ in $t_f J^0 \sim 500$
- Slowing down due to Pauli blocking

# Strongly correlated systems, and many body dark states (?)

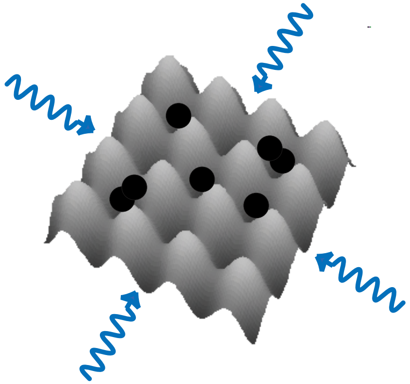
- above scheme works well for (essentially) non-interacting systems
- strongly correlated systems
  - cooling N atoms with U=0 (tune scattering length a=0)
  - turn U on adiabatically to obtain a strongly correlated state

A. Griessner et al. PRL 2006; NJP 2007

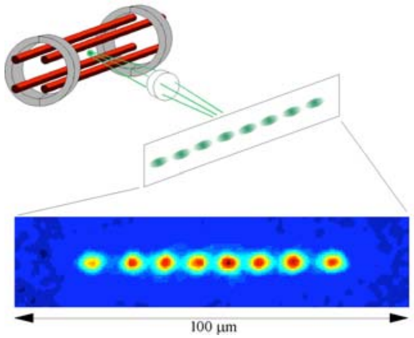
- many-body dark states ?

## Atoms & Ions

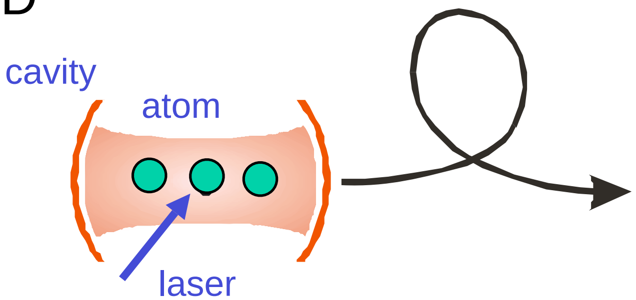
- cold atoms in optical lattices



- trapped ions / Wigner crystals



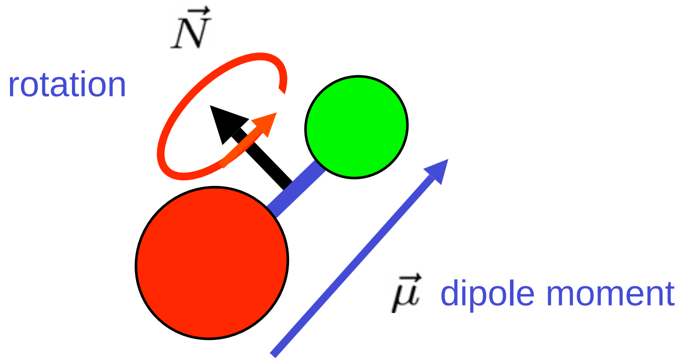

- CQED




- atomic ensembles

## Polar Molecules

- ... in electronic & vibrational ground state




- what's new? ... electric dipole moment
  - couple rotation to DC / AC microwave fields
  - strong dipole-dipole / long range couplings
- ... in addition what we do with cold atoms

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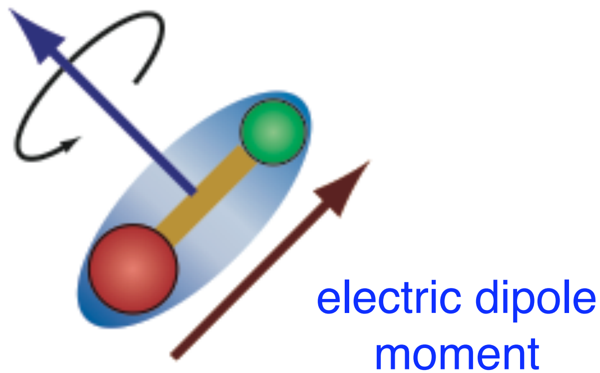
Questions:

- motivation? ... coming experiments
- new physics?

Background material:

# Polar molecules



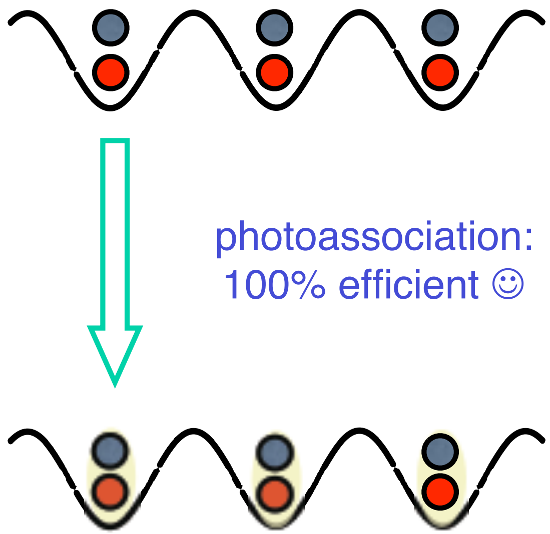
# Preparation of polar molecules in ground state

- Techniques are being developed for ...
  - trapping and cooling
  - generation: photoassociation & buffergas cooling

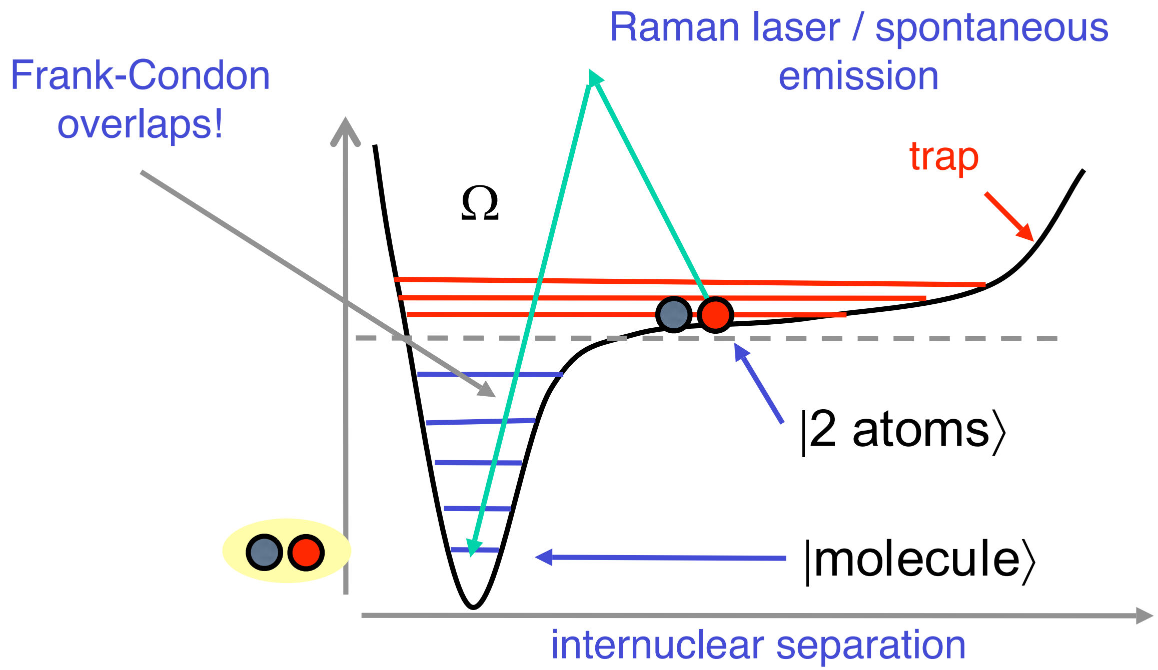
exp: all cold atom labs

exp: Demille, Doyle, Mejer, Rempe, Ye …

Mott insulator:
atoms to molecules



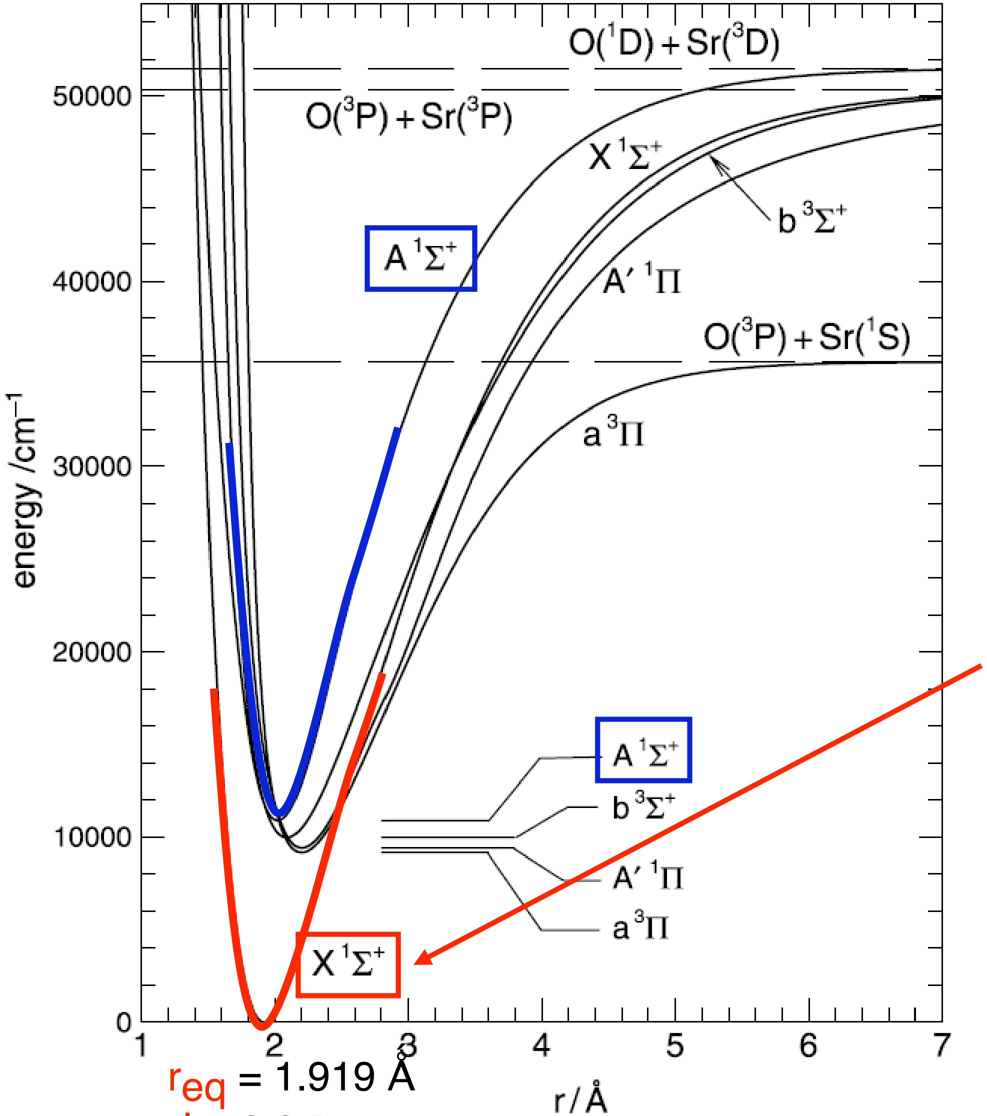

photoassociation




See, e.g., Special Issue on Ultracold Polar Molecules, *Eur. Phys. J. D* **31,** 149–444 (2004).

# Spectroscopy

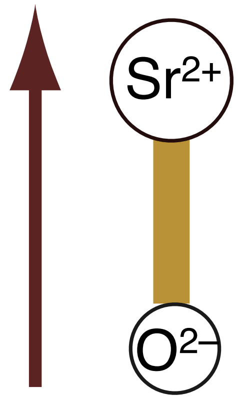
Rydberg-Klein-Rees (RKR)-potentials
(R. Skelton *et al.*, 2003)




$r_{eq}$ = 1.919 Å
d = 8.9 D

heteronuclear molecule with strong <u>persistent</u> 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%) |

<u>$X\ ^1\Sigma^+$ ... electronic groundstate:</u>

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

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

$\omega_{eq}$ = 19.586 THz ... vibrational const.
$B_{eq}$ = 10.145 GHz ... rotational

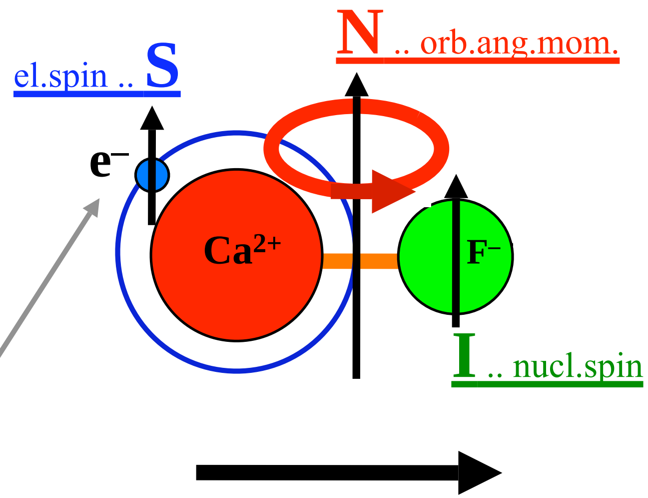
I=0 ... no nuclear momenta for $^{88}$SrO, $^{86}$SrO

# CaF – rotational, fine and hyperfine structure

$X\ ^2\Sigma_{1/2}$ … el. groundstate:

$S=\frac{1}{2}$ ... from open (Ca-)shell
$I=\frac{1}{2}$ ... nuclear momentum (of F)

$r_{eq} = 1.951$ Å ... eq. distance
$\mu_0 = 3.077$ D ... dipole-moment




*electric* dipole moment

strong coupling

talks to optical radiation:
electronic excitations

(like an alkali atom)

talks to microwave radiation:
rotational excitations

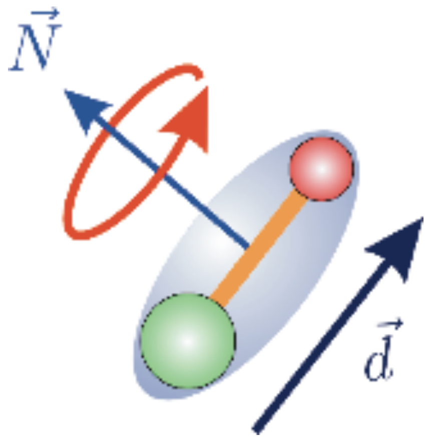
(alkali atom: hyperfine / magnetic)

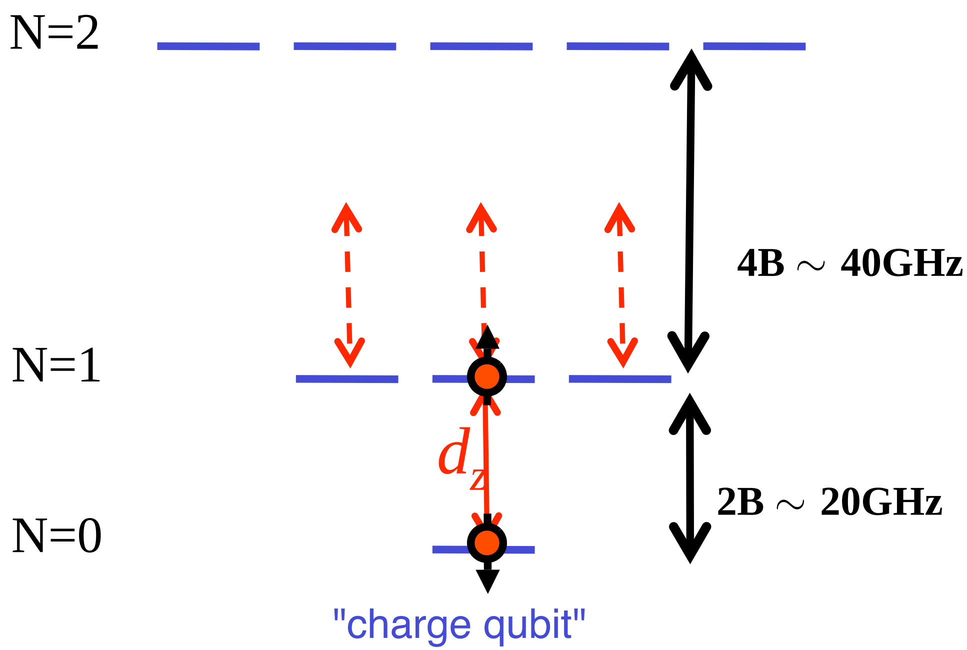
weak couplings :-(

# Single polar molecule I: Rotational spectroscopy

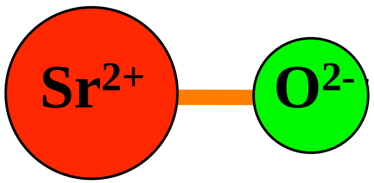
1) Rigid Rotor:

$$H = B\,\mathbf{N}^2$$



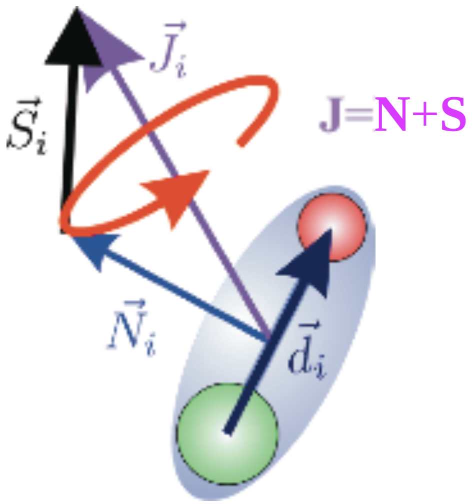

$X^1\Sigma_g^+$ closed shell molecules (SrO, CsRb, … )



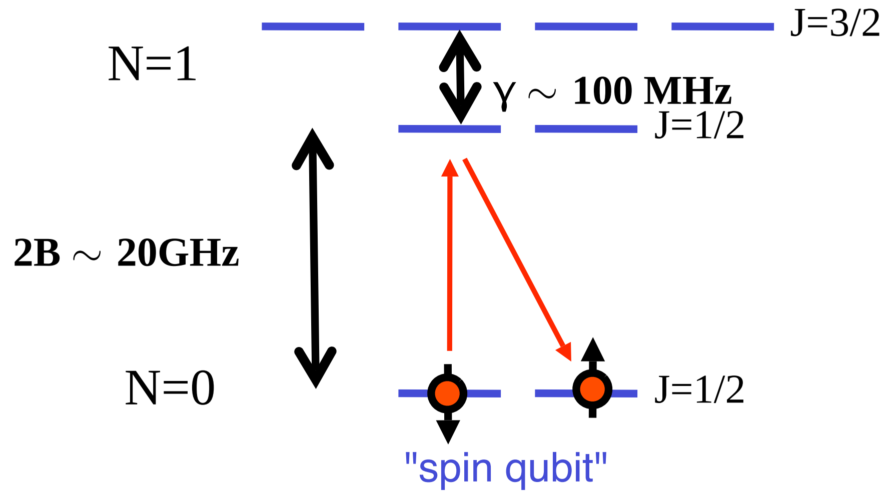

- anharmonic spectrum $E_N = B\,N(N+1)$
- electric dipole transitions $d \sim$ 3-10 Debye
  - microwave transition frequencies
- no spontaneous emission $\Gamma < 0.1$ mHz
  - excited states are "useable"
- encode qubit

# Single polar molecule II: Rotational spectroscopy

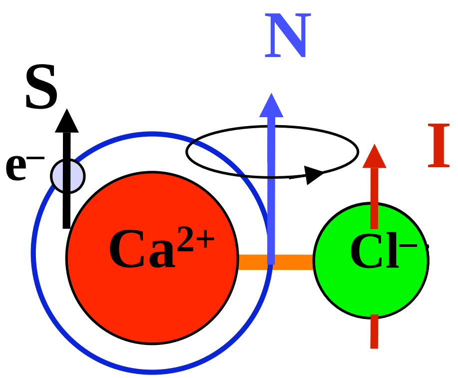
2) Spin Rotation Coupling




$$H = B\,\mathbf{N}^2 + \gamma\,\mathbf{N}\cdot\mathbf{S}$$




$X^2\Sigma_g^+$ molecules with an unpaired electron spin (CaF,CaCl,...)



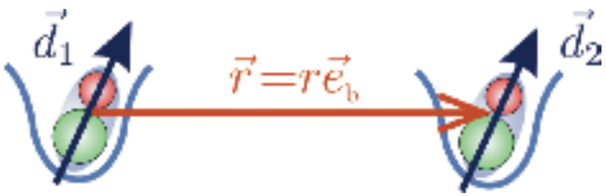

- for e⁻ providing spin degree of freedom
  - encode qubit in rot. ground states
- strong spin-rotational mixing in N>0
  - Raman transitions

---

- for nuclear degree of freedom
  – magnetic trapping, clock states, ...

# Two polar molecules: dipole – dipole interaction

- dipole moment gives rise to interaction of two molecules

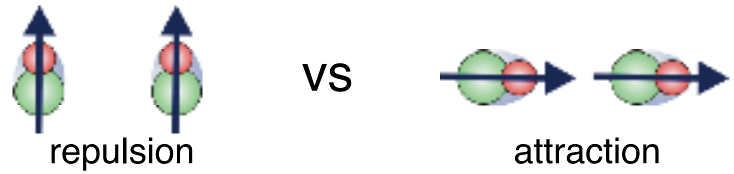



$$V_{\mathrm{dd}} = \frac{\vec{d}_1 \cdot \vec{d}_2 - 3\left(\vec{d}_1 \cdot \vec{e}_b\right)\left(\vec{e}_b \cdot \vec{d}_2\right)}{r^3}$$

features of dipole-dipole interaction

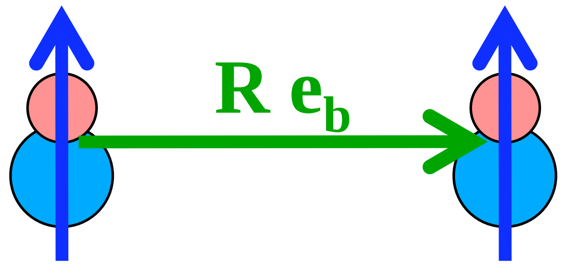
✓ long range $\sim 1/r^3$

✓ angular dependence

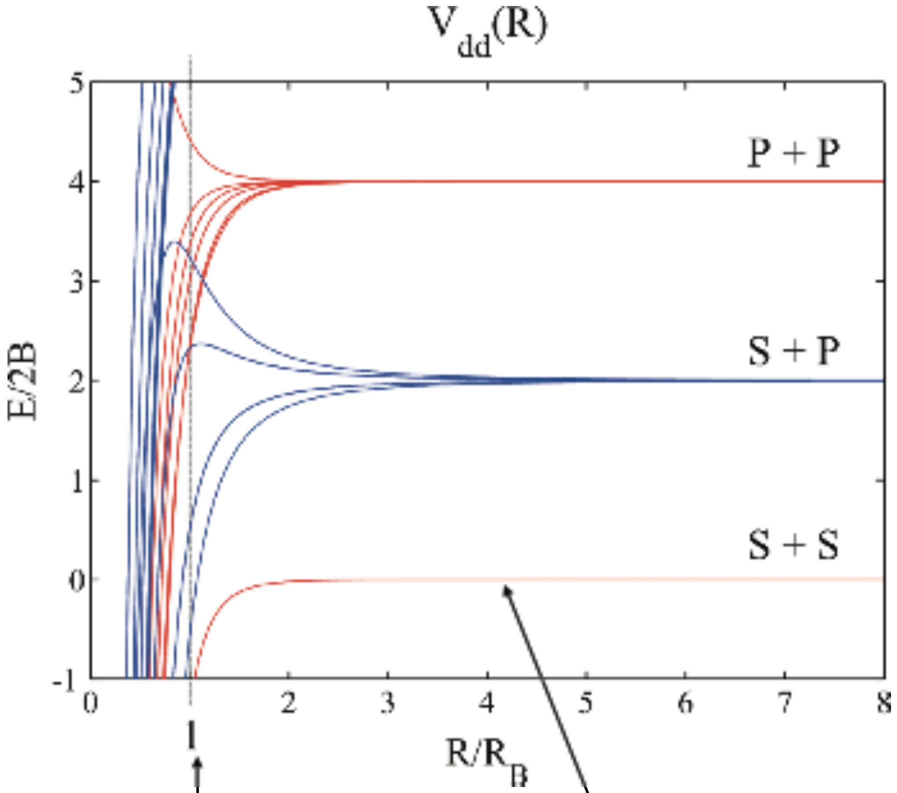


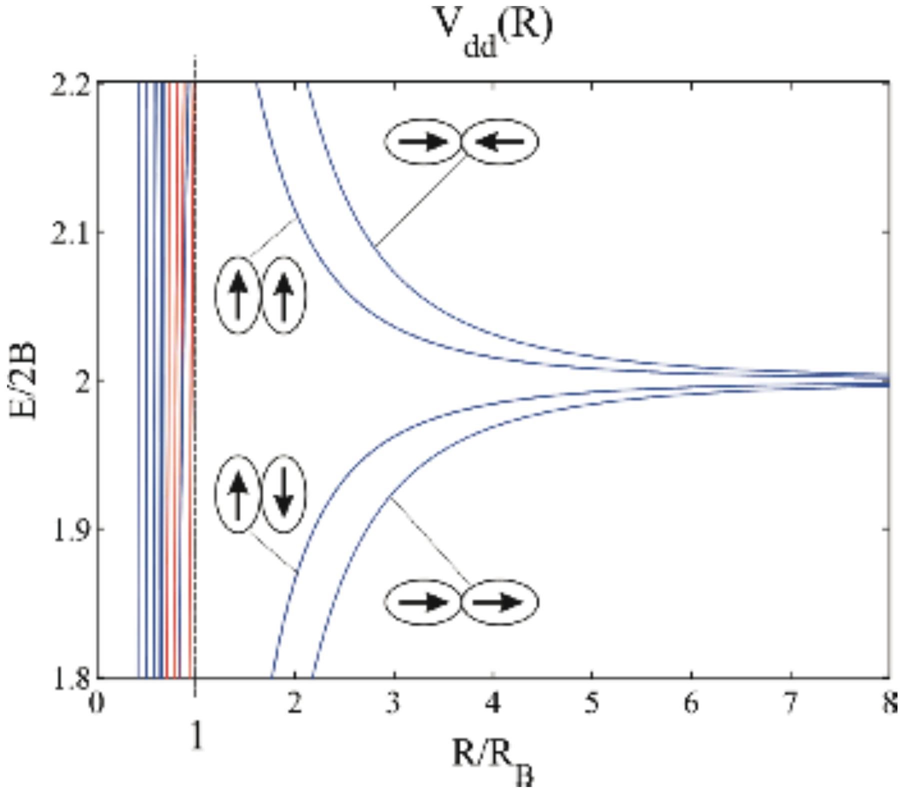

✓ strong! (temperature requirements)

# Adiabatic potentials for two (unpolarized) polar molecules




- **Rotor**



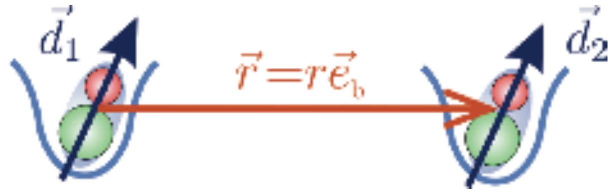

$$R_B = \left(\frac{\mu^2}{3B}\right)^{1/3}$$

$$V_{\rm eff}(R) = -\frac{C_6}{R^6}$$

$$C_6 = \frac{\mu^4}{6B}$$

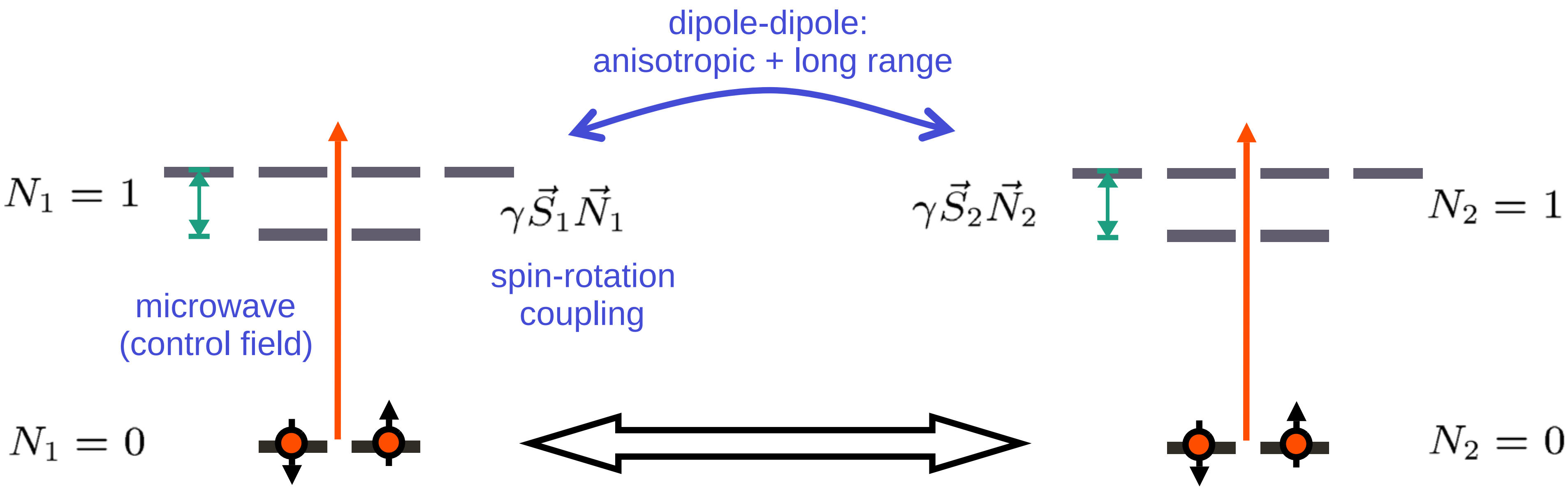
~ 30-60 nm

# Effective Spin-Spin Interactions: qualitative picture




positions fixed by optical lattice

- effective spin-spin coupling: microwave drive + dipole-dipole




Integrating out high energy excitations gives an effective low energy Hamiltonian, we can engineer spin-Hamiltonian

$$H = g \sum_{i \neq j} \sigma_\alpha^{(i)} A^{\alpha\beta}(\vec{x}_i, \vec{x}_j) \sigma_\beta^{(j)}$$

Overview:

Condensed matter and quantum information with cold polar molecules

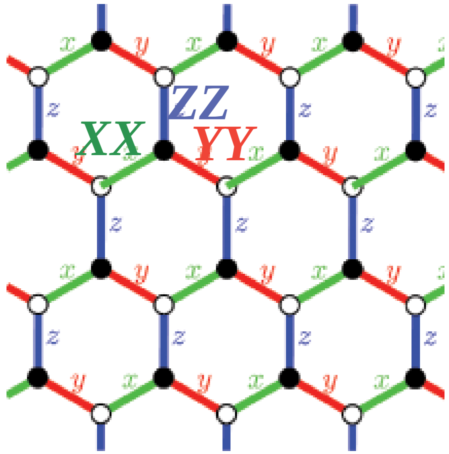
# Condensed matter aspects

- Spin toolbox with cold molecules in optical lattices

$$H_{\text{spin}} = J_\perp \sum_{\text{x-lks}} \sigma_x^i \sigma_x^j + J_\perp \sum_{\text{y-lks}} \sigma_y^i \sigma_y^j + J_z \sum_{\text{z-lks}} \sigma_z^i \sigma_z^j$$

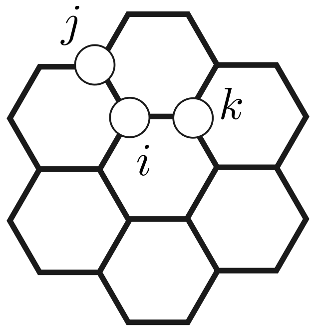
Kitaev model

A. Micheli, G. Brennen, PZ, Nature Physics 2006




- Extended Hubbard models in 1D and 2D in optical lattices

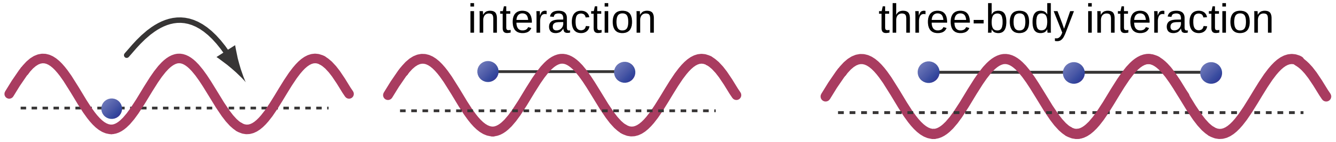
$$H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{1}{2} \sum_{i \neq j} \cancel{U_{ij}} n_i n_j + \frac{1}{6!} \sum_{i \neq j \neq k} W_{ijk} n_i n_j n_k.$$




hopping

*tunable* two-body interaction

*strong repulsive* off-site three-body interaction



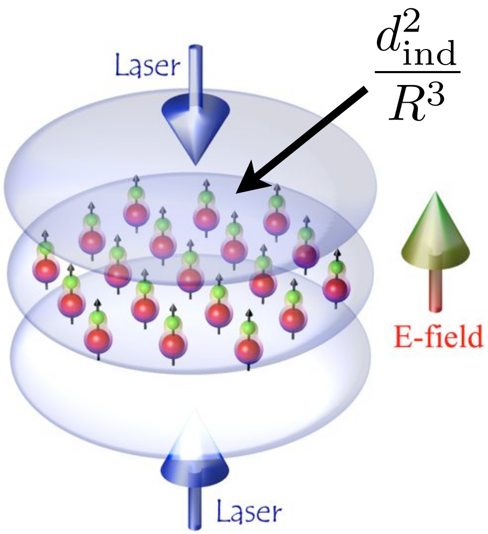
compare: string net Fidkowski et al., cond-mat/0610583

H.P. Büchler, A. Micheli, PZ, preprint

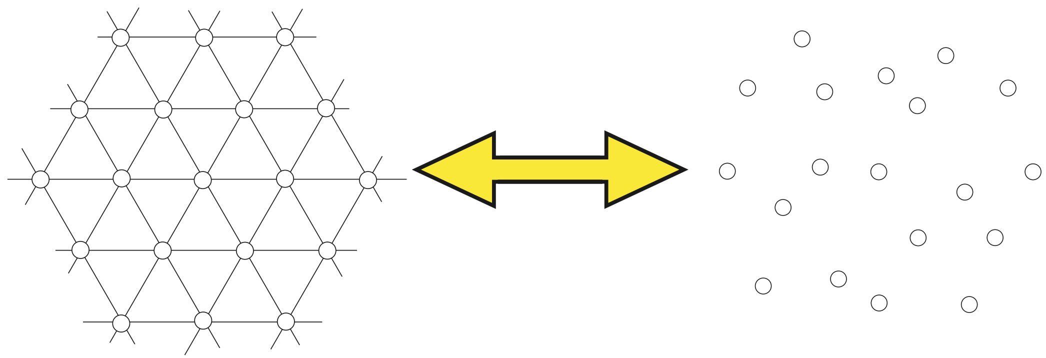
- Self-assembled “dipolar crystals” with cold polar molecules

dipolar crystal:

induced &
aligned dipoles




Quantum melting
- appearance of a crystalline phase
- quantum melting to a superfluid phase



H.P.Büchler, E.Demler, M.Lukin, A. Micheli,
N.V.Prokof'ev, G.Pupillo, PZ, PRL (2007)

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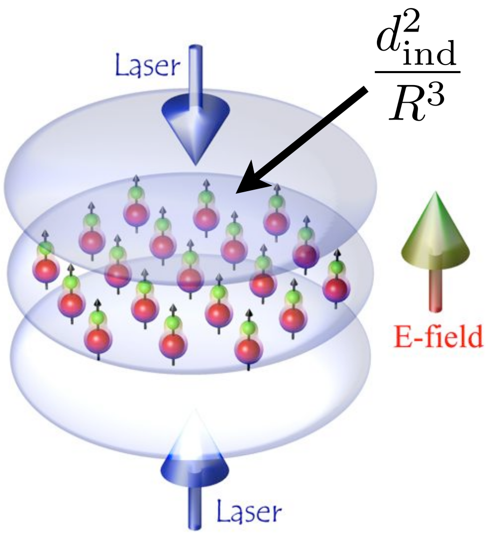
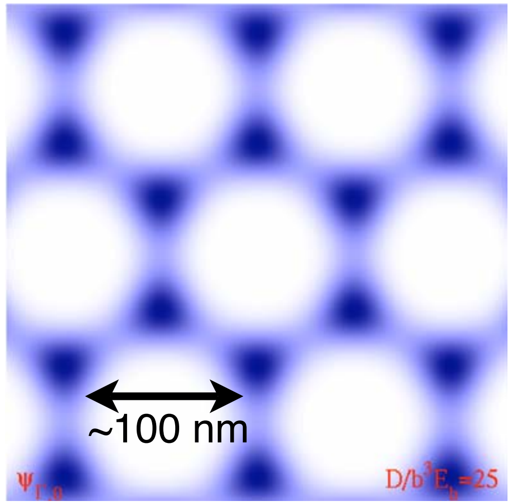



H.P.Büchler, E.Demler, M.Lukin, A. Micheli, N.V.Prokof'ev, G.Pupillo, PZ, PRL (2007)

applications:

atoms in dipolar lattices:
Hubbard models + phonons

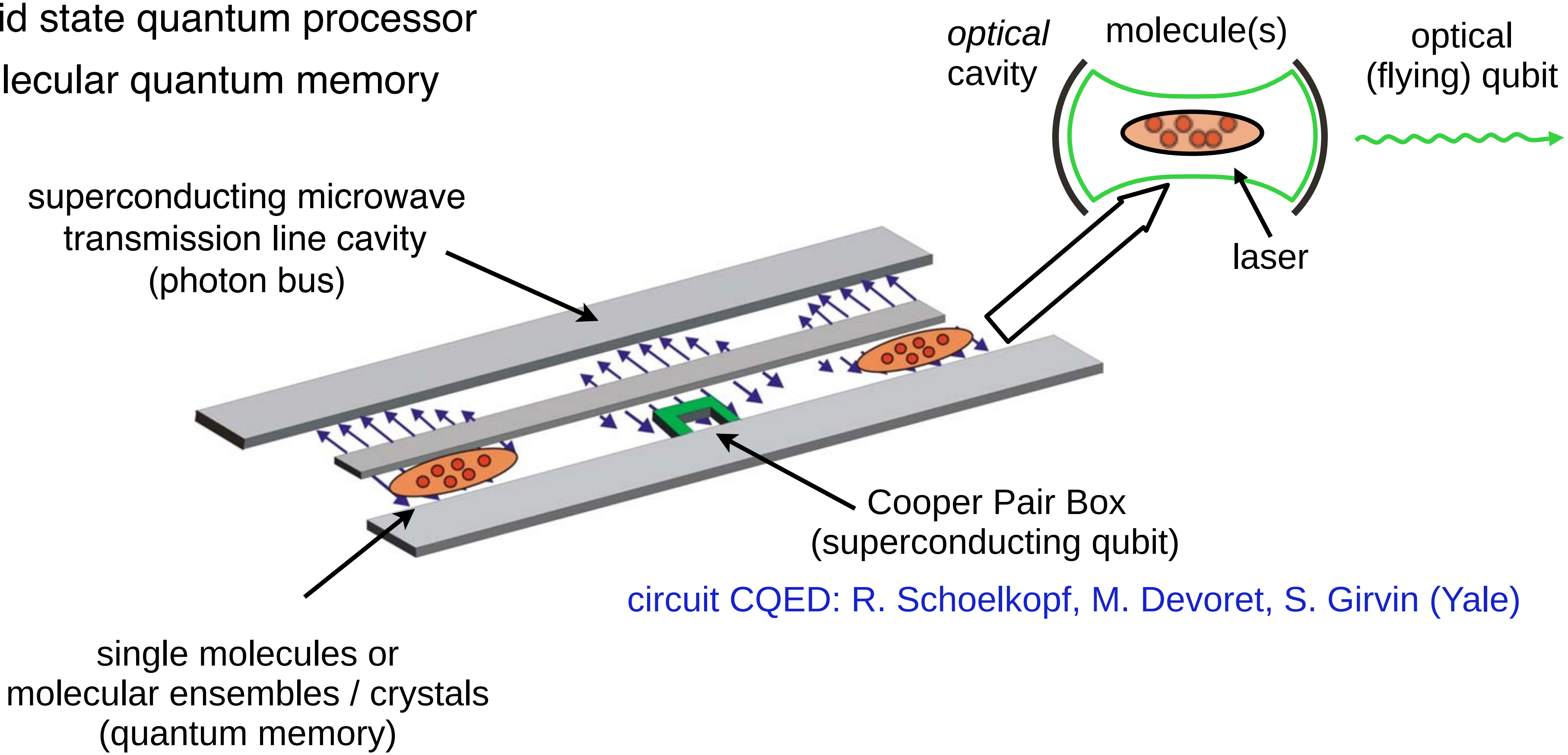



G. Pupillo, M. Ortner et al., work in progress

quantum information:
- memory
- ion-trap type quantum computing

# Quantum information

- AMO - solid state interfaces: hybrid quantum processors
  - solid state quantum processor
  - molecular quantum memory




circuit CQED: R. Schoelkopf, M. Devoret, S. Girvin (Yale)

- Remark: trapping and cooling / read out of molecules close to / via strip line

P.Rabl, D. DeMille, J. Doyle, M. Lukin, R. Schoelkopf and PZ, PRL 2006

A.André, D.DeMille, J.M.Doyle, M.D.Lukin, S.E.Maxwell, P.Rabl, R.J.Schoelkopf, PZ, Nature Physics (2006).

# Three-body interactions & extended Hubbard models

- how to ...
  - generate strong three-body interactions while switching off two-body terms
- extended Hubbard models in 1D and 2D
  - with tunable two body interactions & repulsive three-body
  - phases: example 1D hard core bosons with repulsive three-body terms

H.P. Büchler, A. Micheli, PZ, preprint

We start in the continuum and add the optical lattice later

# Dynamics with n-body interactions

- Hamiltonians of condensed matter physics are effective Hamiltonians, obtained by integrating out the high energy excitations

$$H = \sum_i \left( \frac{\mathbf{p}_i^2}{2m} + V_{\mathrm{T}}(\mathbf{r}_i) \right) + V_{\mathrm{eff}}\left(\{\mathbf{r}_i\}\right)$$

effective interaction

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

usually small corrections

two particle interaction

three particle interaction

example: He

- Hamiltonians with three-body interactions
  - ground states with exotic phases & excitations (topological, spin liquids etc.)
  - difficult to find examples in nature (Fractional Quantum Hall Effect, ... AMO?)

# Dynamics with n-body interactions

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turn off (?)

two particle interaction

three particle interaction

strong & repulsive (?)

- Cold gases of atoms and molecules
  - we know the high energy degrees of freedom & manipulate by external fields
  - Q.: switch off two-body, while generating strong repulsive three-body (?)

... with polar molecules dressed by external fields
(without introducing decoherence)

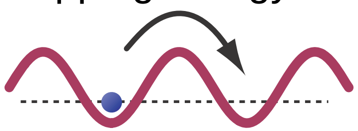
# Hubbard models with three-body interactions

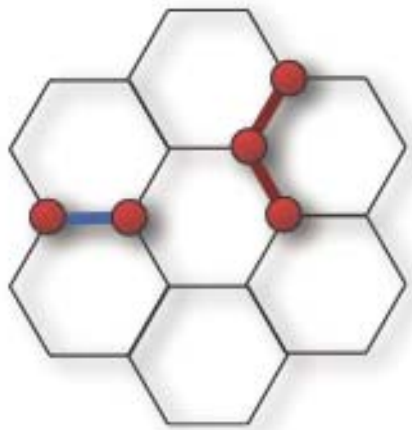
- Rem.: Typical Hubbard models with polar molecules involve strong dipole-dipole (two-body) offsite interactions
- Extended Hubbard models in 1D and 2D

+ small next-nearest neighbor interactions

$$H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{1}{2} \sum_{i \neq j} \cancel{U_{ij} n_i n_j} + \frac{1}{6!} \sum_{i \neq j \neq k} W_{ijk} n_i n_j n_k .$$

hopping energy | two-body interaction | three-body interaction





- strong three-body interaction

$$W/J \sim 0 ... 30$$
$$J \sim 0.1 E_r$$

- tunable two-body interaction

$$U/J \sim -300 \,...\, 300$$

# Hubbard models with three-body interactions

- Rem.: Typical Hubbard models with polar molecules involve strong dipole-dipole (two-body) offsite interactions

- Extended Hubbard models in 1D and 2D

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$$H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{1}{2} \sum_{i \neq j} \cancel{U_{ij} n_i n_j} + \frac{1}{6!} \sum_{i \neq j \neq k} W_{ijk} n_i n_j n_k .$$

hopping energy | two-body interaction | three-body interaction

---

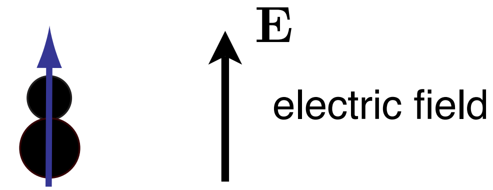
- Rem.: effective higher-order interactions are also obtained from a Hubbard models in J/U-perturbation theory ...
  - example: tJ-model
  - however, these effective interactions are necessarily small

# How to calculate effective n-body interactions ... basic idea

- Step 1: “dressed” single polar molecule

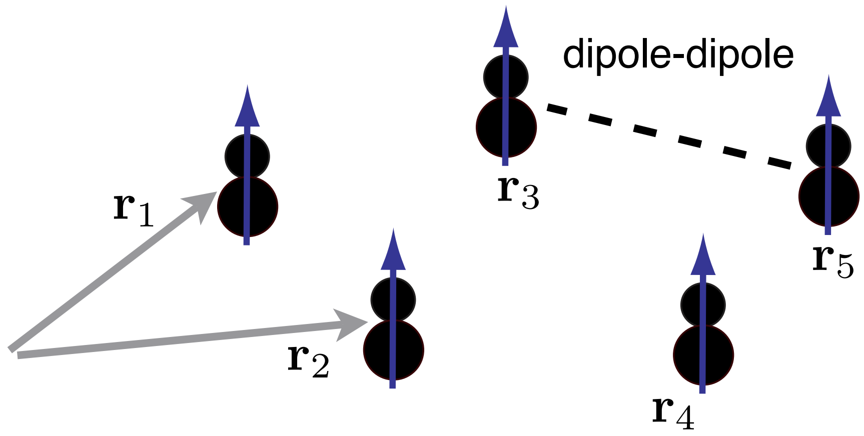
  We dress molecules prepared in the ground state by adiabatically switching on AC / DC electric fields.

polar molecules




- Step 2: interaction between molecules

  For fixed positions of the molecules we adiabatically switch on dipole-dipole interactions.




We identify the interaction energy

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

... with the interaction potential in the spirit of a Born-Oppenheimer approximation.

Our goal is now (i) to choose a molecular setup and (ii) calculate the BO potential.

We choose the following setup ...

## Step 1: Single molecule as an effective spin-1/2

- Single molecule as a “spin-1/2 in an effective magnetic field”

Two-level System

- in rotating frame / RWA

$$H_0^{(i)} = \frac{1}{2}\begin{pmatrix} \Delta & \Omega \\ \Omega & -\Delta \end{pmatrix} = \mathbf{h}\mathbf{S}_i$$

- dressed eigenstates

$$|+\rangle_i = \alpha|g\rangle_i + \beta|e,1\rangle_i$$
$$|-\rangle_i = -\beta|g\rangle_i + \alpha|e,1\rangle_i$$

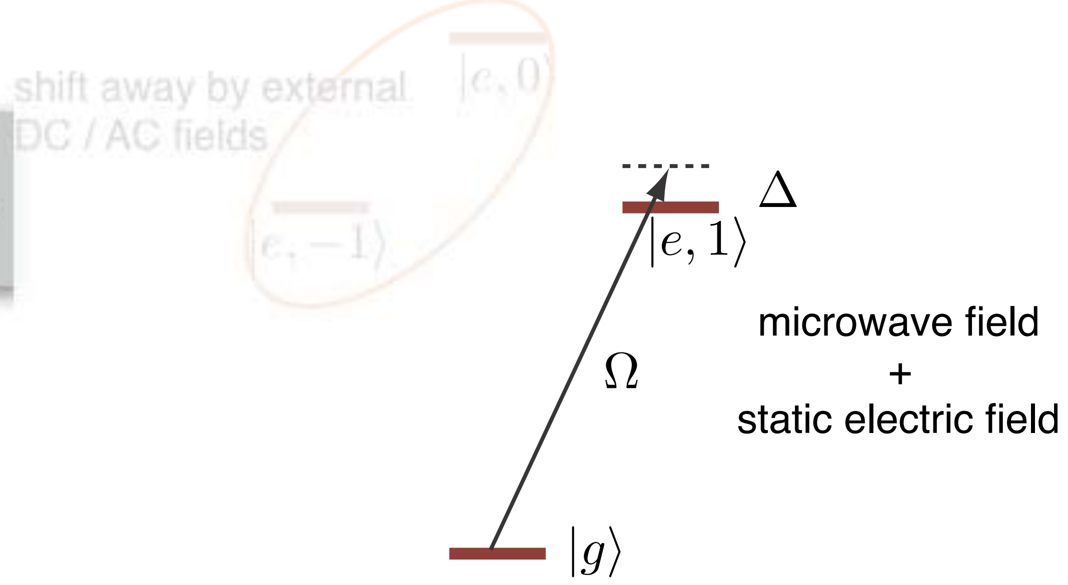
and energies

$$E_\pm = \pm\sqrt{\Omega^2 + \Delta^2}/2$$

- adiabatically turning on AC field

$$|g\rangle_i \rightarrow |+\rangle_i \quad (\text{for } \Delta > 0)$$

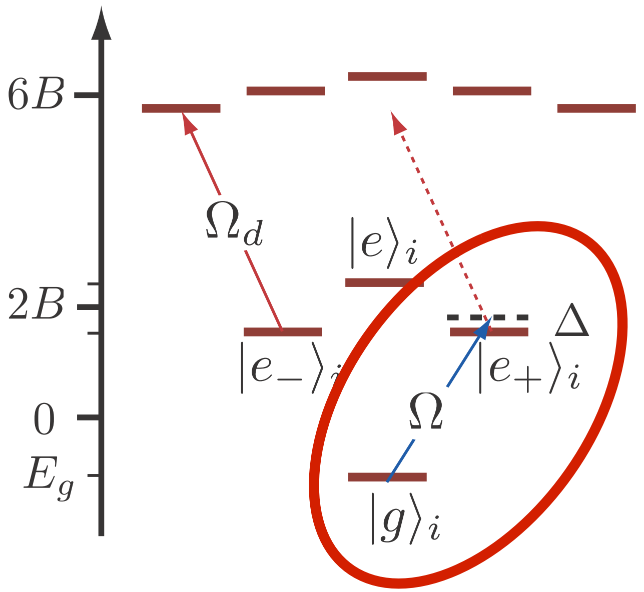
rotation spectrum:




- induced static dipole moments due to the static electric field

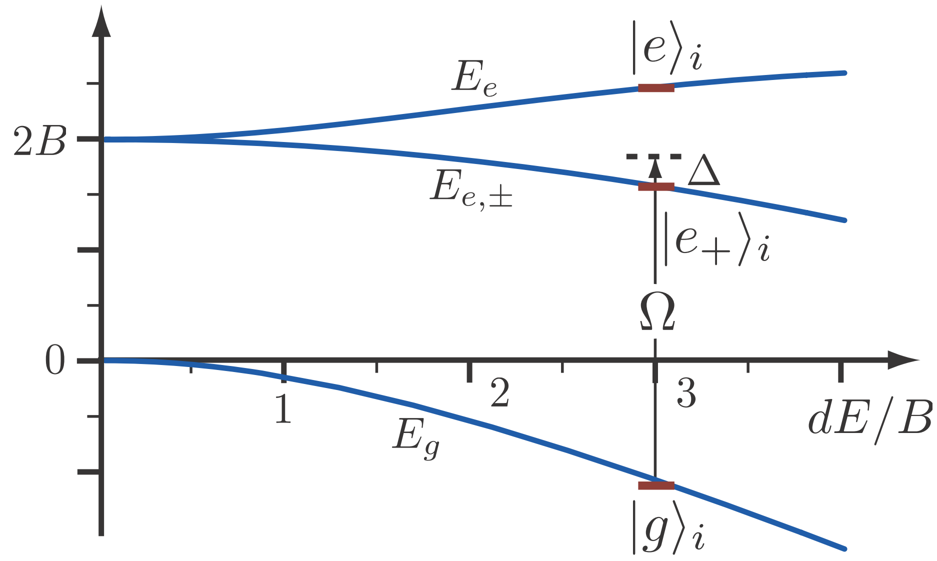
Details ...

- rotational spectrum in AC & DC field




two-level system

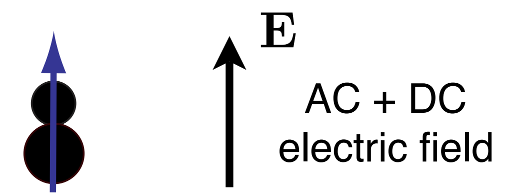
- DC field




- induced static dipole moments due to the static electric field

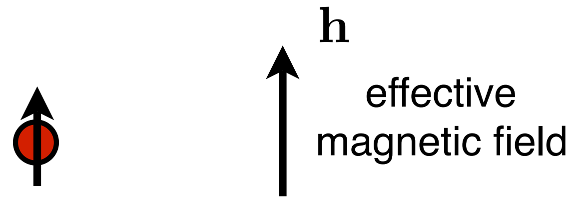
# Convenient mapping: (fixed) molecules to (fixed) spin-1/2

- Single molecule



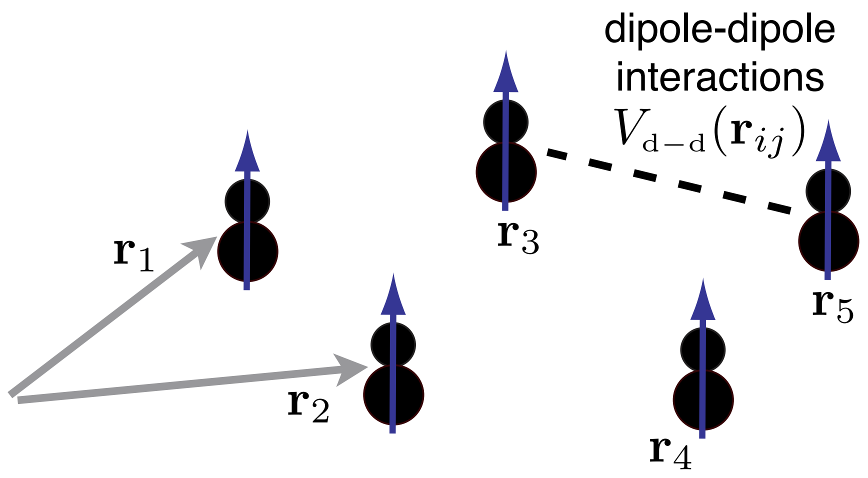

$$H_{\mathrm{rot}}^{(i)} = B\mathbf{N}_i^2 - \mathbf{d}_i\mathbf{E}(t)$$

- Spin-1/2 in magnetic field

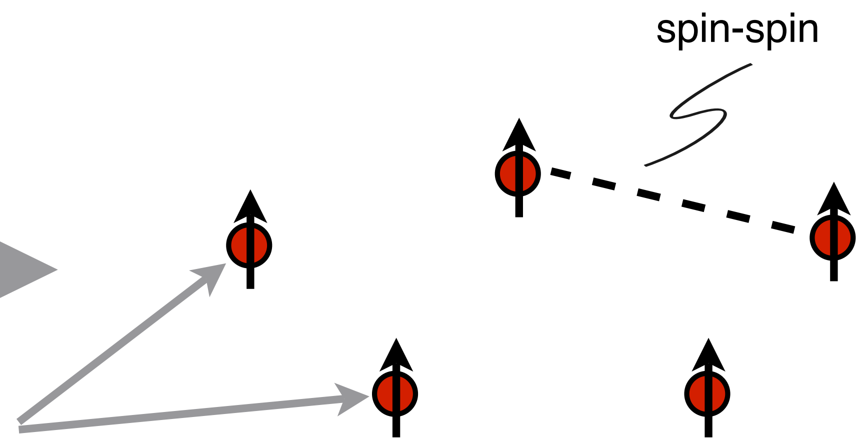



$$H_0^{(i)} = \mathbf{h}\mathbf{S}_i$$

- Interacting (fixed) molecules



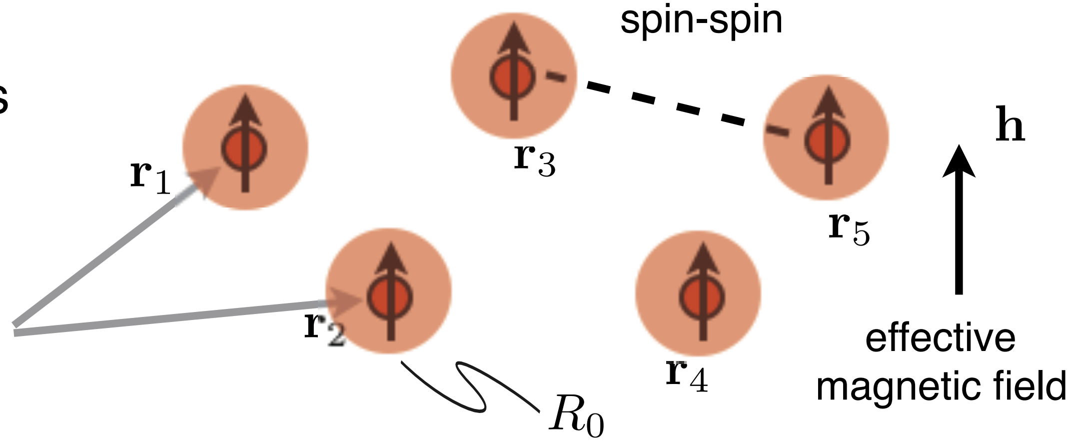

- Interacting (fixed) spins




Our goal is to calculate the energy for fixed $\{\mathbf{r}_i\}$, i.e. the Born-Oppenheimer potential $V_{\mathrm{eff}}(\{\mathbf{r}_i\})$. This is conveniently done in the spin-picture.

# Step 2: Interactions

- Ensemble of (static) molecules as interacting spins in magnetic field




Dipole-dipole interaction

- in rotating frame / RWA

$$H = \sum_i \mathbf{h}\mathbf{S_i} + \sum_{i \neq j} D\left[(\cdots)(S_i^x S_j^x + S_i^y S_j^y) - (\cdots)S_i^z S_j^z + (\cdots)S_i^z\right]$$

dipole-dipole interaction $\nu(\mathbf{r}) = \dfrac{1-\cos\theta}{r^3}$

XXZ- model in a magnetic field

- Paramagnetic phase $\mathbf{h} >> D/a^3$ or $D/(a^3|\mathbf{h}|) = (R_0/a)^3 << 1$

weakly interacting regime:
interaction potential in perturbation theory

mean distance

- Provided $|\mathbf{r}_i - \mathbf{r}_j| > R_0$ we can calculate the interaction energy perturbatively

# Interaction energy (= Born Oppenheimer potential)

## Interaction energy

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

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

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

(iii) Perturbation theory to calculate the interaction energy

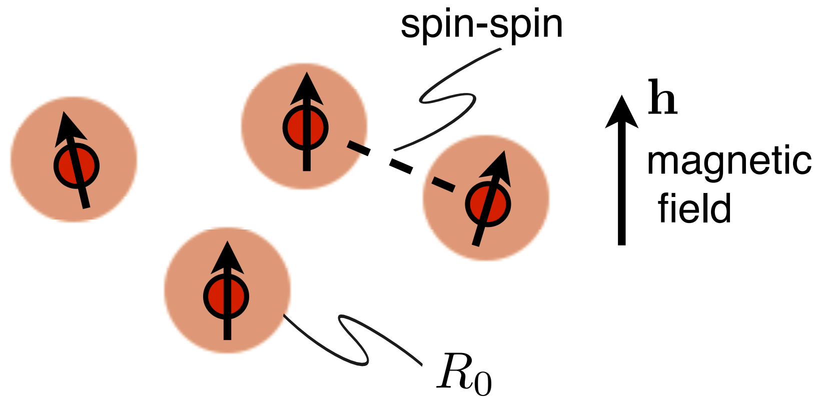
$$\Pi_i |+\rangle_i \to |G\rangle$$

$$E^{(1)}(\{\mathbf{r}_i\}) = \dots$$

$$E^{(2)}(\{\mathbf{r}_i\}) = \dots$$

valid for:

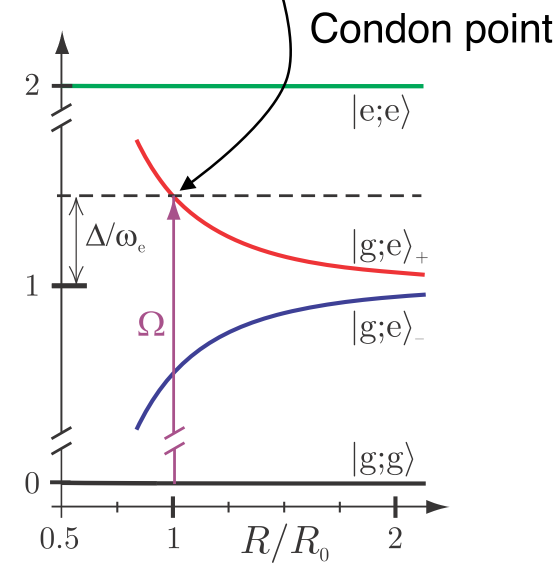
$$|\mathbf{r}_i - \mathbf{r}_j| > R_0$$



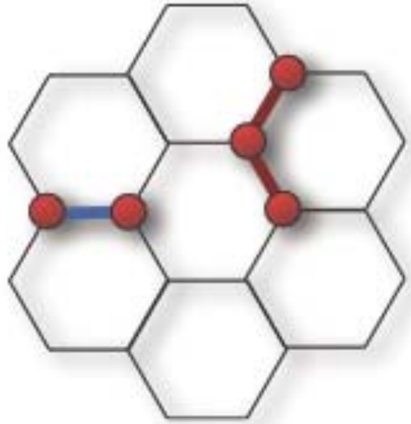

“weak” dipole interaction for ...

$$\frac{D}{\sqrt{\Delta^2 + \Omega^2}} = R_0^3 \ll a^3$$

interparticle distance



# Extended Hubbard model



- Hamiltonian:

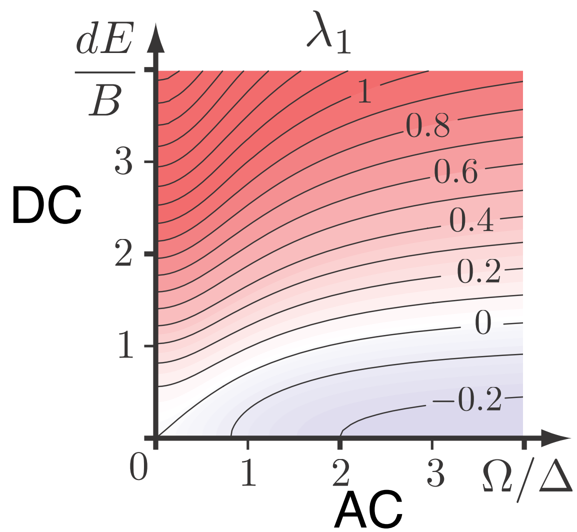
$$H = -J\sum_{\langle ij\rangle} b_i^\dagger b_j + \frac{1}{2}\sum_{i\neq j} U_{ij} n_i n_j + \frac{1}{6!}\sum_{i\neq j\neq k} W_{ijk} n_i n_j n_k.$$

- two-body interaction

$$U_{ij} = U_0 \frac{a^3}{|\mathbf{R}_i - \mathbf{R}_j|^3} + U_1 \frac{a^6}{|\mathbf{R}_i - \mathbf{R}_j|^6}$$

$U_0 = \lambda_1 D/a^3$ repulsive

tunable




- three-body interaction

$$W_{ijk} = W_0 \left[\frac{a^6}{|\mathbf{R}_i - \mathbf{R}_j|^3 |\mathbf{R}_i - \mathbf{R}_k|^3} + \text{perm}\right].$$

repulsive

- hard core onsite condition ... $a_0 \ll R_0 \ll \lambda/2$

# 1D hard core Boson with three-body

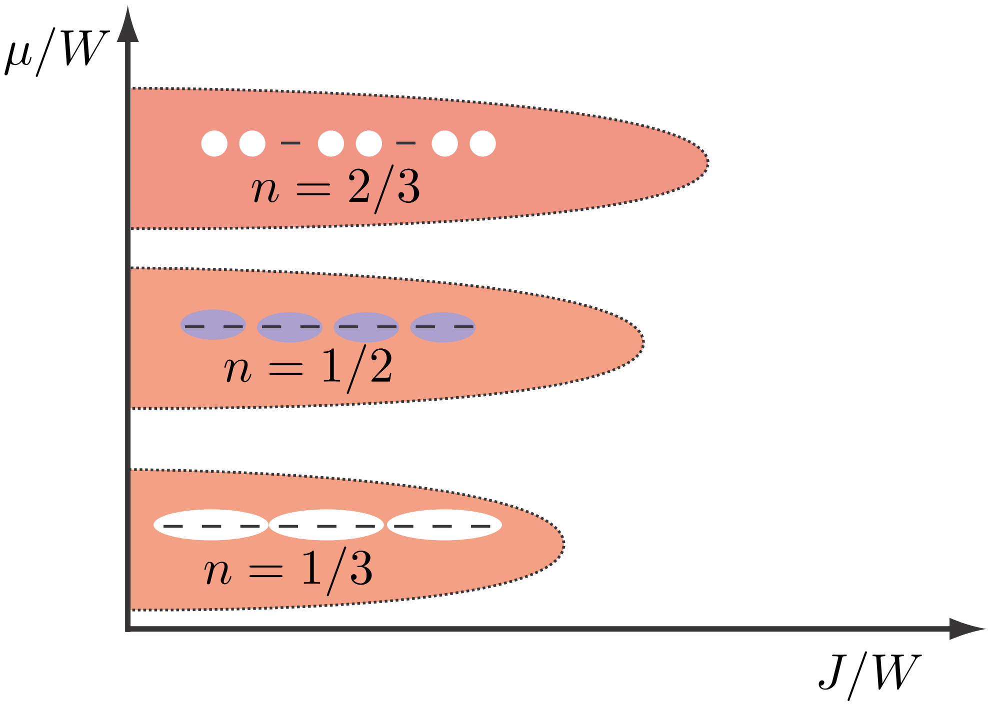
$$H = -J\sum_i \left[b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i\right] + W\sum_i n_{i-1}n_i n_{i+1}$$

## Bosonization

- hard-core bosons
- instabilities for densities:

$n = 2/3 \quad n = 1/2 \quad n = 1/3$

- quantum Monte Carlo simulations (in progress)




## Critical phase

- algebraic correlations
- compressible
- repulsive fermions

## Solid phases

- excitation gap
- incompressible
- density-density correlations

$$\langle \Delta n_i \Delta n_j \rangle$$

- hopping correlations (1D VBS)

$$\langle b_i^\dagger b_{i+1} b_j^\dagger b_{j+1} \rangle$$