

## \* POLAR LATTICE GASES

• Up to this point, we have assumed that the particles interact via short-range isotropic potentials. There's however a new generation of experiments in which another type of interaction, namely the dipole-dipole interaction plays a crucial role. This is in particular the case of magnetic atoms (Cr, Dy, Er) and polar molecules (as  $\text{K Rb}$ ,  $\text{RbCs}$ ,  $\text{NaK}$ , etc.)

• Let's comment first briefly about magnetic atoms. Typical alkali atoms have a magnetic moment of  $\sim \mu_B$ . There are however other atoms with a much larger magnetic moment, this is in particular the case of Cr ( $6\mu_B$ ), Er ( $7\mu_B$ ) and Dy ( $10\mu_B$ ). Interestingly all these systems have been brought to quantum degeneracy (for both the fermionic and the bosonic isotopes).

• Bose-Einstein condensates of magnetic atoms present interesting properties induced by the dipole-dipole interaction (we will have a look to the peculiar features of the dipole-dipole interaction momentarily). Some of these funny properties include:

- Stability depends on the trap geometry
- Excitations present a roton-like minimum (not yet observed)
- Dipole-induced spin relaxation

and more (see experiments, especially by Pfau's group (Stuttgart), Labushe's group (Paris Nord), Iv's group (Berkeley) and Ferlaino's (Innsbruck)).

• Degenerate dipolar Fermi gases have also interesting properties including the recently observed deformation of the Fermi surface, (experiment at F. Ferlaino's group in Innsbruck, 2019).

• Recent experiments at F. Ferlaino's group have succeeded in the magnets-association of weakly-bound Er<sub>2</sub> molecules. (Basically by ramping across a Feshbach resonance, which due to the complex scattering in Er occur for many low-B values)

\*  $\text{Fe}_2$  molecules have a maximal magnetic moment of  $14 \mu_B$  [the actual values created in current experiments are somewhat smaller,  $\sim 12 \mu_B$ ]. This large magnetic moment and the doubled mass make this molecules very dipolar [the "dipolarity" may be quantified by the so-called dipolar length  $a_d = m \mu_B \mu^2 / \mu_0 \mu^2$ , which scales as  $\sim m \mu^2$ ]. Remarkably, this value is comparable to that attainable with KRb molecules (see below). ~~¶~~

\* There's however a clear difference.  $\text{Fe}_2$  is a weakly-bound homonuclear molecule in a highly-excited vibrational level. On the contrary KRb (or other polar molecules) are deeply-bound heteronuclear molecules in the absolute ground state, as we will see below.

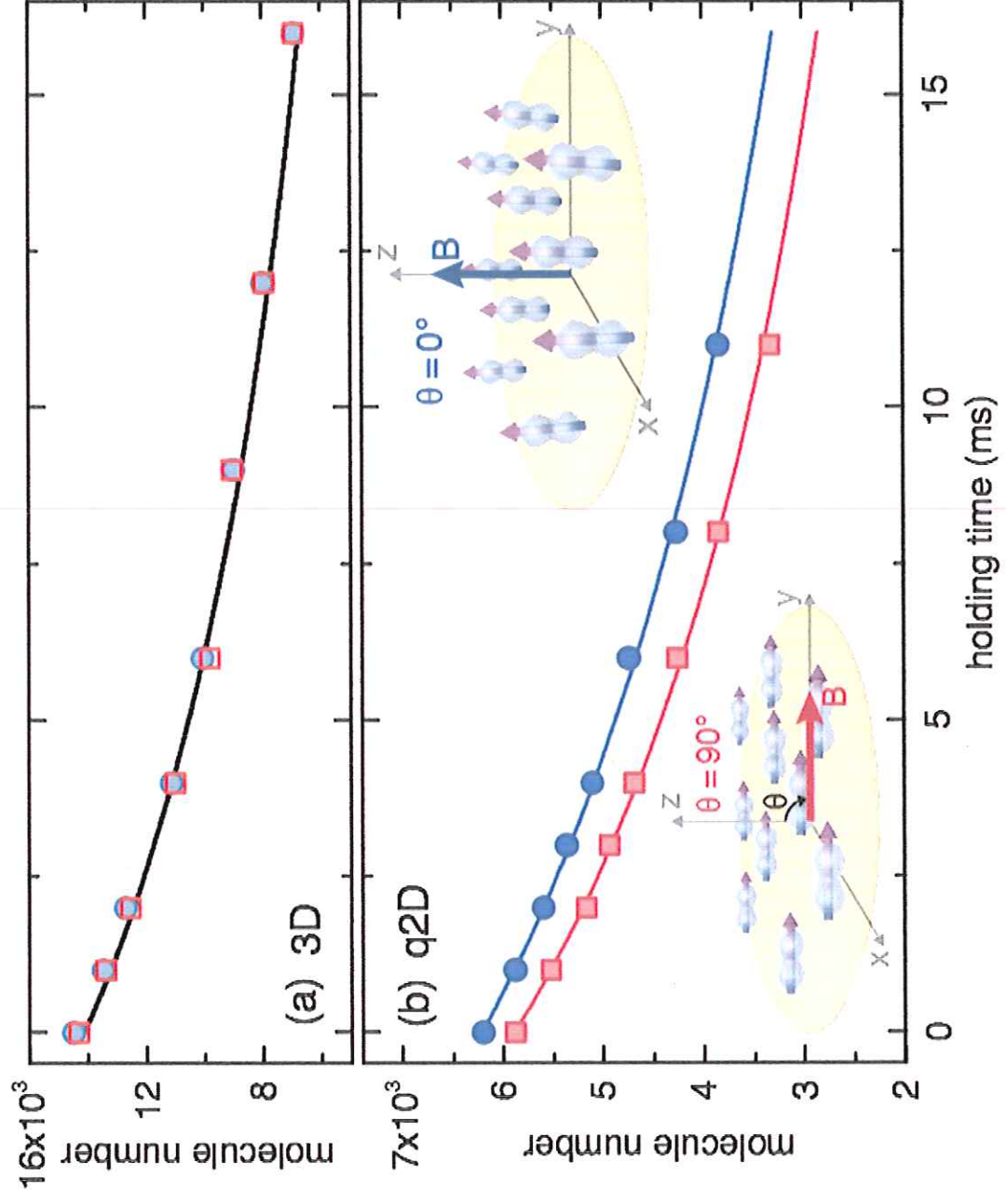
\* In the recent experiments in Innsbruck [Frisch et al, arXiv: 1504.04578] they have probed this "dipolarity" by studying losses in 3D and quasi-2D traps (see p. 120)

Whereas in 3D traps losses are independent of the dipole orientation [this losses occur due to vibrational quenching into lower-lying molecular states], in quasi-2D the decay rate depends clearly on the dipole orientation with respect to the plane. This is because if the dipole is perpendicular to the plane then the dipole-dipole interaction is repulsive in all directions in the plane, shielding the molecules against approaching too close.

\* I will not comment much more on magnetic atoms, since I'll focus mostly on polar molecules. But we should be aware of progresses on magnetic atoms (and molecules) which may be also relevant under some conditions for lattice gases.

# Dipolar effects in $\text{Er}_2$ molecules

[Firsch et al., arXiv:1504.04578]



- Let's move now to polar molecules, which may present large electric dipole moments, much larger than atomic magnetic dipoles.
- A polar molecule is maximally polar when placed into its lowest ro-vibrational state. This has been done in ~~the~~ pioneering KRB experiments at JILA (at D. Jin's group) by a combination of

- (i) First forming weakly-bound molecules associated from ultracold atoms via Feshbach resonances
- (ii) Subsequently coherently transfer into the ground ro-vibrational state via a 2-photon stimulated rapid adiabatic passage (STIRAP) (see p. 122, where we show actually the case of NaK experiments at MIT)

• KRB molecules are however problematic, because they are unstable against 2-body collisions, since the reaction  $KRB + KRB \rightarrow K_2 + Rb_2$  is energetically allowed. This may be solved (at least partially) in quantum due to the dipole-dipole repulsion (similarly as what we discussed above about  $Er_2$  experiments).

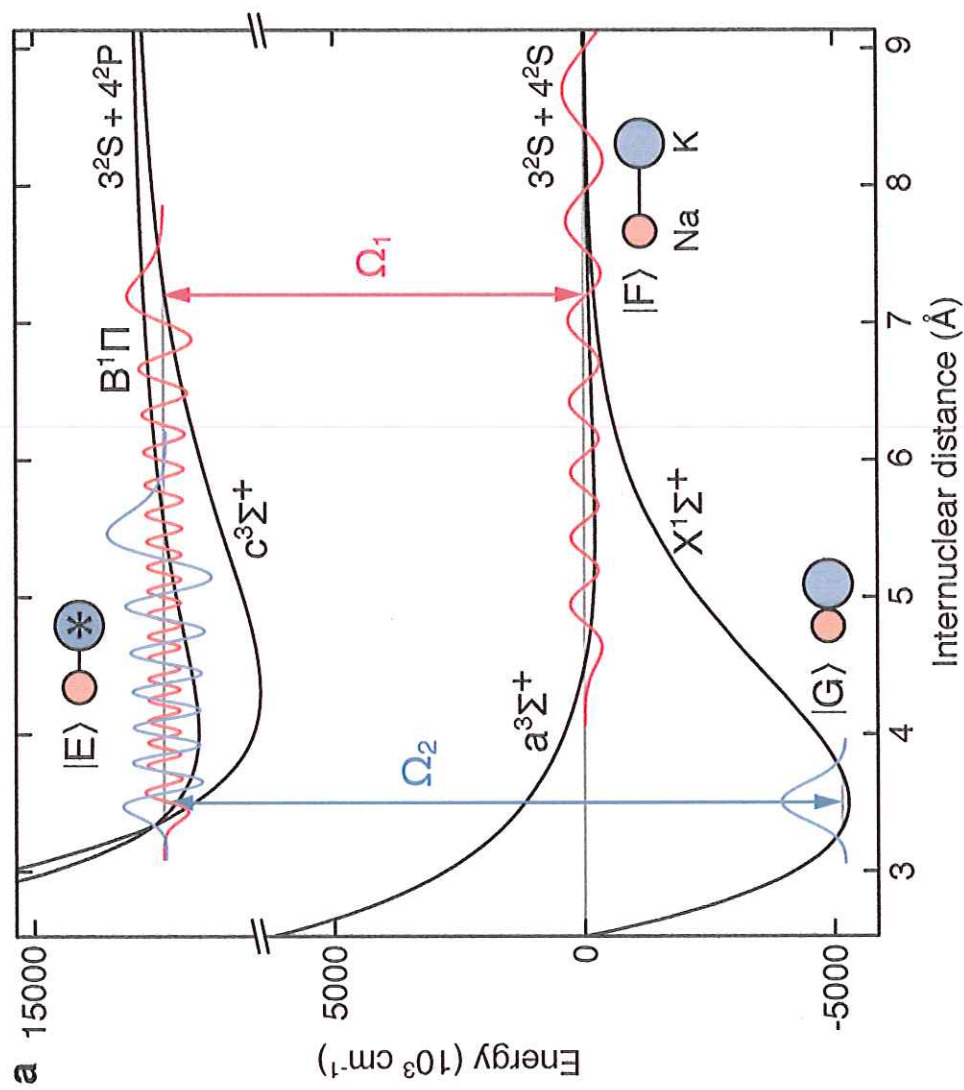
• Fortunately not all molecules are reactive. This is in particular the case of RbCs and NaK.

Recently RbCs has been transferred to the ground ro-vibrational state in experiments in H.C. Nägerl's lab in Innsbruck, and of S. Cornish's lab in Durham. (RbCs is bosonic)

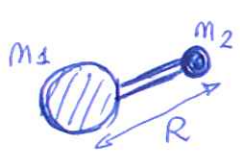
Also  $^{23}Na^{40}K$  (which is fermionic) has been transferred to the lowest ro-vibrational state in very recent experiments at M. Zurolev's lab at MIT. The spin-polarized (nearly quantum degenerate) molecular gas has a lifetime of 2.5 seconds, highlighting NaK's stability against 2-body chemical reactions.

• Placing the molecules in the lowest ro-vibrational state is important because the dipole moment is maximal there. However, this dipole is in the molecular frame. The molecule must be oriented in the laboratory frame by an external electric field. Let's understand this important point.

# Formation of molecules in the lowest ro-vibrational state



\* let's consider a simple rigid-rotor model of diatomic molecules.



$$\hat{H}_{rot} = B \hat{J}^2$$

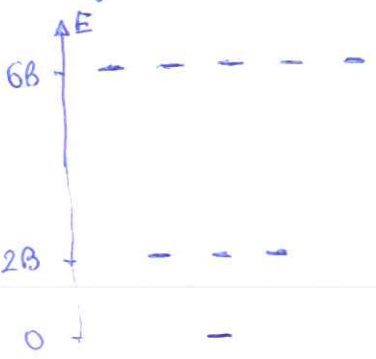
$\hat{J} \equiv$  molecule angular momentum operator (in  $\hbar$  units)

$$B = \frac{\hbar^2}{2\mu R^2} \equiv \text{rotational constant}$$

$R \equiv$  equilibrium internuclear distance  
 $\mu \equiv$  reduced mass

[\* Note: Molecules with large mass differences, as LiCs, have small reduced mass ( $\mu_{LiCs} \approx m_{Li}$ ), hence  $B$  is large; This makes more difficult to orient them, as we will see right now].

\* The eigenstates of  $\hat{H}_{rot}$  are the rotational states  $|J, m_J\rangle$  with energies  $B J(J+1)$ , and degeneracy  $2J+1$ .

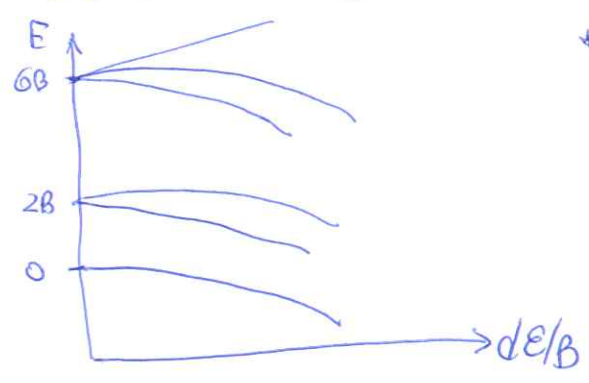


\* This degeneracy is lifted in the presence of an external field  $\vec{E} = E \vec{e}_z$ , which leads to a Stark shift.

$$\hat{H} = \hat{H}_{rot} - d E \cos \Theta$$

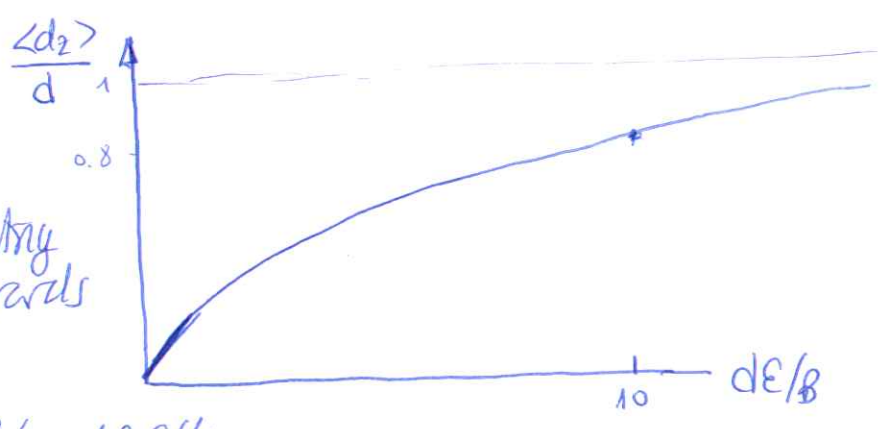
where  $\Theta$  is the angle between the electric field orientation ( $z$  here) and the internuclear axis.

\* The Stark shift admixes the different rotational states



\* We may then obtain the average dipole moment (now in the laboratory frame)

$$\langle d_z \rangle = d \langle \cos \Theta \rangle = - \frac{dE_0}{dE}$$



\* The dipole moment increases linearly for small  $dE/B$ , saturating asymptotically for  $dE/B \gg 1$  towards the bare value  $d$ .

\* For typical values of  $d \sim 10$ ,  $B/h \sim 100$  GHz then  $dE/B \sim 1$  for 10 kV/cm, which is large but accessible.

[Note: in the recent MIT experiments on NaK, a field of 2 kV/cm was applied to get 0.8 Debye, the bare dipole is 2.72 Debye, hence  $\frac{\langle d_z \rangle}{d} \approx 0.3$ .]

\* So, the admixture of rotational states induced by the electric field is crucial, without it there's no effective dipole.

[Note: Note, however, that I could admix rotational states in an alternative way. I could transfer part of the population from  $|J=0, M_J=0\rangle$  to  $|J=1, M_J=\pm 1, 0\rangle$ . The upper rotational state and the lowest one will have now a non-zero dipolar term  $\Rightarrow \langle J=1, M_J=0 | d_z | J=0, M_J=0 \rangle \Rightarrow \langle 1, 0 | Y_{10} | 0, 0 \rangle \neq 0$  whereas  $\langle 0, 0 | Y_{10} | 0, 0 \rangle = 0$ , obviously by selection rules. The latter shows us in an alternative way, why we need to admix rotational states to get an effective dipole  $\langle d \rangle$ ].

\* So polar molecules allow for 2 control knobs of the dipole-dipole interaction:

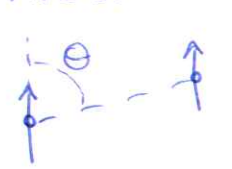
(i) the strength of the orienting field controls the dipole strength, which may range from zero to dipole moments of the order of the Debye ( $1 \text{ Debye} \equiv 3.3 \times 10^{-30} \text{ C}\cdot\text{m}$ )

(ii) The direction of the orienting field determines the orientation of the dipoles.

Note that (ii) is also there for magnetic atoms, in which the direction of the magnetic field  $\vec{B}$  determines the orientation of the dipoles. On the contrary in magnetic atoms the magnetic dipole exists even in absence of the magnetic field (this opens interesting questions about the physics of unaligned magnetic dipoles at zero magnetic field).

\* As for the moment, polar molecules in the ro-vibrational ground state have not been brought to quantum degeneracy, although it seems reasonable to expect that this may be achieved soon.

• Let's have now a look to the dipole-dipole interaction between two dipoles oriented along z:



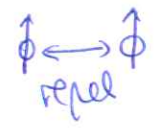
$$V_{dd}(\vec{r}) = \frac{d^2}{4\pi\epsilon_0} \left( \frac{1-3\cos^2\theta}{r^3} \right)$$

d = electric dipole

(Note: for magnetic atoms, instead of  $\frac{d^2}{4\pi\epsilon_0}$  one writes  $\frac{\mu_0\mu^2}{4\pi}$ , with  $\mu$  the magnetic moment.)

• The dipole-dipole interaction presents two key features when compared to the van-der-Waals-like interaction we have considered up to now:

- It is long-range → it depends as  $1/r^3$  and not as  $1/r^6$  as the vdw interaction
- It is anisotropic → due to the  $(1-3\cos^2\theta)$  factor



• As already mentioned the dipole-dipole interaction has crucial consequences for the physics of Bose-Einstein condensates and of degenerate Fermi gases. Some of them have been already observed experimentally, as already discussed in p. 118.

• Here we will be particularly concerned about the physics of polar lattice gases.

Let's consider dipolar bosons in an optical lattice. ~~They~~ We will assume, as we did for most of the course, that the particles just occupy the lowest band.



The system is then described by the Hamiltonian

$$\hat{H} = \int d^3r \hat{\Psi}^\dagger(\vec{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + \frac{1}{2} \int d^3r' U(\vec{r}-\vec{r}') \hat{\Psi}^\dagger(\vec{r}') \hat{\Psi}(\vec{r}') \right] \hat{\Psi}(\vec{r})$$

where  $U(\vec{r}) = g \delta(\vec{r}) + V_{\text{dd}}(\vec{r})$

[Note: The actual interparticle interaction may be substituted by the simple pseudopotential  $U(\vec{r})$ , where  $g = 4\pi\hbar^2 a/m$ , but in principle  $a = a(d)$ . This dependence may manifest itself quite dramatically in the so-called shape resonances, at which the scattering length diverges. The previous pseudopotential has been shown to be valid away from shape resonances.]

We may now proceed as in p. 6. We expand in the basis of Wannier functions

$$\hat{\Psi}(\vec{r}) = \sum_{\vec{j}} w_{\vec{j}}(\vec{r}) \hat{a}_{\vec{j}}$$

and assume tight-binding (i.e. very poorly overlaps between wavefunctions at different sites).

If we do so we find an effective lattice Hamiltonian, which has again a Bose-Hubbard form but with intersite interactions

$$\hat{H} = -t \sum_{\langle \vec{j}, \vec{j}' \rangle} \hat{a}_{\vec{j}}^\dagger \hat{a}_{\vec{j}'} + \frac{U_0}{2} \sum_{\vec{j}} \hat{n}_{\vec{j}} (\hat{n}_{\vec{j}} - 1) + \sum_{\vec{\delta}} \frac{U_{\vec{\delta}}}{2} \sum_{\vec{j}} \hat{n}_{\vec{j}} \hat{n}_{\vec{j}+\vec{\delta}}$$

→ Extended Hubbard model

where  $t \equiv - \int d^3r w_{\vec{j}}^*(\vec{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) \right] w_{\vec{j}'}(\vec{r})$

$$U_0 \equiv g \int d^3r |w_{\vec{j}}(\vec{r})|^4 + \iint d^3r d^3r' |w_{\vec{0}}(\vec{r})|^2 |w_{\vec{j}}(\vec{r}')|^2 V_{\text{dd}}(\vec{r}-\vec{r}')$$

$$U_{\vec{\delta}} \equiv \iint d^3r d^3r' |w_{\vec{0}}(\vec{r})|^2 |w_{\vec{j}+\vec{\delta}}(\vec{r}')|^2 V_{\text{dd}}(\vec{r}-\vec{r}')$$

\* We should compare this Hamiltonian with the Bose-Hubbard Hamiltonian of p. 127

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• As in there, we have on-site interactions. Note however that they result from the interplay between short-range and dipolar interactions:  $U_0 \equiv U_0^{(sc)} + U_0^{(cd)}$

• The main new ingredient is the presence of intersite interactions, which result exclusively from the dipole-dipole interaction.

(Note: A caveat here. In the derivation of the extended Hubbard model we have forgotten some terms which may become relevant for large dipoles, in particular collisionally-induced tunneling terms of the form  $a_i^\dagger (\hat{n}_j + \hat{n}_j^\dagger) a_{j\pm}$ .)

\* Few further comments about the "control knobs" concerning the extended Bose-Hubbard model:

\* Due to the anisotropy of the dipolar interaction, the spatial dependence of the on-site wavefunction may significantly modify  $U_0^{(cd)}$ . One may e.g. get  $U_0 = 0$  but  $U_{0\pm} \neq 0$  by playing with this (and perhaps also Feshbach resonances).

\* In  $2D$  <sup>and 1D</sup> lattices one may modify the orientation of the dipoles with respect to the plane (line), hence modifying the amplitude and even the sign of  $U_0$ .

\* Note that  $U_0$  decays with  $\delta$  (for zero-dimensional sites as  $1/\delta^3$ ). This means that under proper conditions of lattice spacing and relatively weak dipole one may reduce just to nearest neighbors ( $\delta = 1$ ).

(Note: However for large dipoles interaction to many neighbors may play an important role.)

\* Intersite interactions

\* As mentioned above, the most relevant novel feature of polar lattice gases is provided by the existence of intersite interactions.

\* The effects of intersite interactions have been observed in BEC experiments [we will discuss an even more compelling direct observation of intersite interactions in the strongly correlated regime].

Let me briefly comment on the BEC experiments performed with <sup>52</sup>Cr in Stuttgart at T. Pfau's group (Müller et al., PRA 84, 053601 (2011))

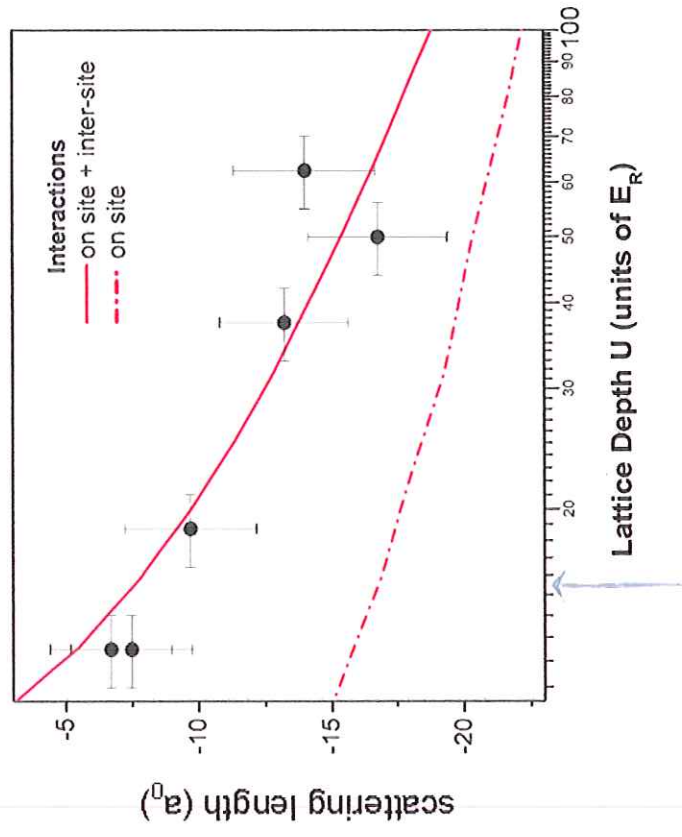
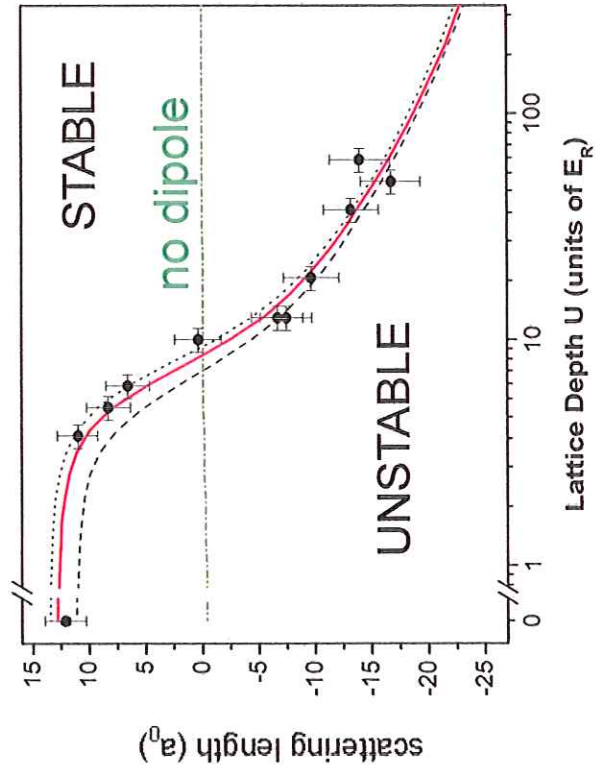
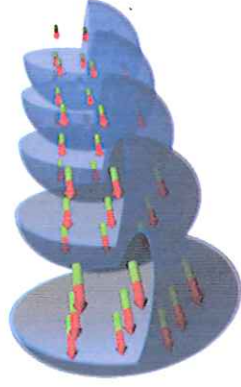
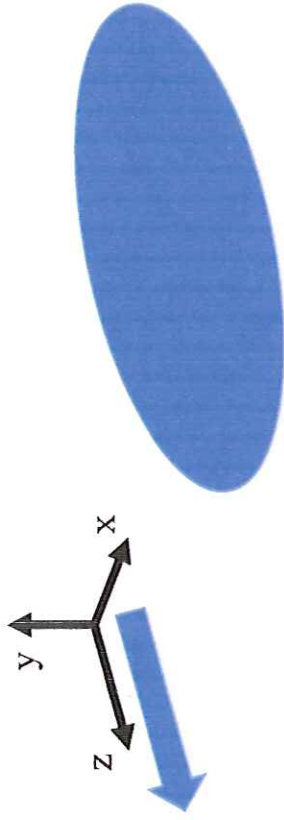
• In these experiments ~~a~~ BEC of <sup>52</sup>Cr was confined in a cigar-shaped trap with its axis along the dipole orientation. ~~A~~ 1D lattice was overlaid along the ~~trap~~ trap axis (see p. 129).

• In absence of the lattice, the dipoles are in the cigar-like trap, where they see each other (in average) head-to-tail. As a result the dipole-dipole interaction is ~~in average~~ negative (i.e. attractive). That's a problem for the stability of the BEC (against collapse). One needs a positive scattering length such that the short-range repulsive interactions compensate the dipolar attraction.

• In the experiment they measure the optical scattering length  $a_{sc}$  (note that for  $a < a_0$  the system is unstable) as a function of the lattice depth. <sup>(see p. 129)</sup> When the lattice depth increases  $a_{sc}$  decreases. This is expected, because on-site the cloud is basically a parallel where dipoles see each other, in average, side by side, and hence the dipole-dipole interaction is repulsive. Hence one needs eventually a negative scattering length to destabilize the system (i.e.  $a_{sc}$  becomes eventually negative.)

# Stability of dipolar BECs in 1D optical lattices

[Müller et al., PRA 84, 053601 (2011)]



The crucial point <sup>here</sup> is that the critical ac is also affected by intersite interactions, even when the hopping between layers is basically zero! Since intersite interactions are mostly head-to-tail they tend rather to destabilize the system. This is why ac is less negative than what one would assume without taking into account intersite interaction (see p. 129).

\* Interestingly, as mentioned above, intersite interactions are there, even if the hopping vanishes. This opens the interesting possibility of inducing energy transfer (i.e. the transfer of excitations) even when matter is not actually transferred (since the hopping is zero!)

\* This is easy to understand without entering in too much detail. We may take e.g. 2 condensates separated by a large barrier such that hopping between them vanishes. Then, if we displace one of the condensates, or create a density perturbation in one of them, we will modify intersite interactions which hence induce a dynamics in the other condensate. We have transferred excitations without transferring matter!

\* For the case of BECs this means that Bogoliubov excitations are actually shared between the 2 condensates. The excitations are 3D even if the BECs cannot move from their quasi 2D planes!

\* We will see later even a more clear <sup>experimental</sup> proof of intersite dipole-dipole interaction.

## \* Extended Hubbard model

- let's come back to the extended Hubbard model of p. (126).
- For the non-dipolar case we recover the usual Bose-Hubbard Hamiltonian of p. (9), which as we already know is characterized by two distinct ground-state phases: superfluid and Mott insulator.
- The presence of the inter-site interactions leads to a much richer physics, which I will briefly (and incompletely) review now.

## \* Crystals and supersolids

- let's consider a 2D lattice (i.e. we assume a strong alignment along the 3<sup>rd</sup> direction, say  $z$ ). The dipoles are oriented along  $z$ . As a result the inter-site interactions are side-by-side, and hence repulsive.

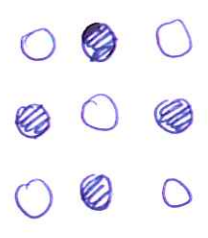
As a result, if the inter-site repulsion is large enough, the particle density may present a modulation different from that of the lattice. That's easy to understand, if the nearest-neighbor interaction is very strong, and I can place the particles 2 sites apart, then I will do it, forming in this way a crystal.

These crystals are characterized by modulated density-density correlations  $\langle n_{\vec{r}} n_{\vec{r}'} \rangle$ , and are hence revealed by peaks in the so-called structure factor, which is nothing else than the Fourier transform of the density-density correlations

$$S(\vec{k}) \Rightarrow \sum_{\vec{r}, \vec{r}'} e^{i\vec{k} \cdot (\vec{r} - \vec{r}')} \langle n_{\vec{r}} n_{\vec{r}'} \rangle$$

If there's a crystal-like modulation then  $S(\vec{k})$  presents a peak.

• For example, in a square lattice at half-filling the system may enter for sufficiently large  $U_2$  an insulating checker-board pattern, characterized by a peak of  $S(\vec{u})$  at  $\vec{u} = (\pi, \pi)$



\* Other lattice geometries, dipole orientations and filling factors may lead to other crystalline patterns.

\* Interestingly, an even more intriguing phase may occur, in which the system remains superfluid but the density presents a modulation (i.e. there's both off-diagonal long-range order,  $\rho_{ij} \equiv \langle \psi_i^\dagger \psi_j \rangle \xrightarrow{|\vec{r}-\vec{r}'| \rightarrow \infty} \text{constant}$ , and a peak in  $S(\vec{u})$ ).

This peculiar phase is called a Supersolid

[Note: Quantum Monte Carlo calculations have shown that a supersolid may be stabilized against phase separation (i.e. against separation in crystal and superfluid) for  $\langle n \rangle > 1/2$  and  $U_3 > U_0/2$ , where  $z$  is the number of neighbors; see Sengupta et al., PRL 94, 207202 (2005).]

\* Another interesting phase has been discussed for 1D polar lattice bosons. Let's consider a filling  $\langle n \rangle = 1$ . If  $U_0$  is large enough we may just consider possible occupation  $n = 0, 1, 2$ . One may then introduce a pseudospin (in a similar way as we did in p. 30)

$$S^z = n - \langle n \rangle = -1, 0, 1 \quad [\text{we will call } \delta n_j = n_j - \langle n \rangle = n_j - 1]$$

The system becomes then to a large extent equivalent to a spin-1 gas with extended interactions (so-called spin-1 Haldane chain). Such a spin chain may present an intriguing phase in which  $S^z = \pm 1$  appear in alternating order along the chain separated by strings of  $S^z = 0$  of arbitrary length; something like

fluo: ... (+1) 0 0 ... 0 (-1) 0 0 ... 0 (+1) 0 ... 0 (-1) 0 ... 0 (+1) ...

Translated into bosonic language flu would be something like this:



This phase is characterized by the so-called string order (which resembles the parity order we discussed in p. 129)

$$\Theta_S^2 \equiv \lim_{|i-j| \rightarrow \infty} \langle \delta n_i (-1)^{\sum_{k>i} \delta n_k} \delta n_j \rangle \neq 0$$

This phase appears for intermediate values of  $U_0$  and  $U_1$  between a Mott insulator and a density-wave phase (i.e. between a phase (1111...) and a phase (2020...)) → see p. 134.

and receives the name of Haldane insulator

[see Dalla Torre et al., PRL 97, 260401 (2006)]

• let me finish this brief incomplete review about novel phases in dipolar gases with a short comment about intersite Composites. Intersite-~~interactions~~ interactions may bound particles belonging to different sites. This introduces the funny possibility of observing interlayer superfluids, i.e. superfluids formed by pairs of particles belonging to different layers in a 1D lattice.

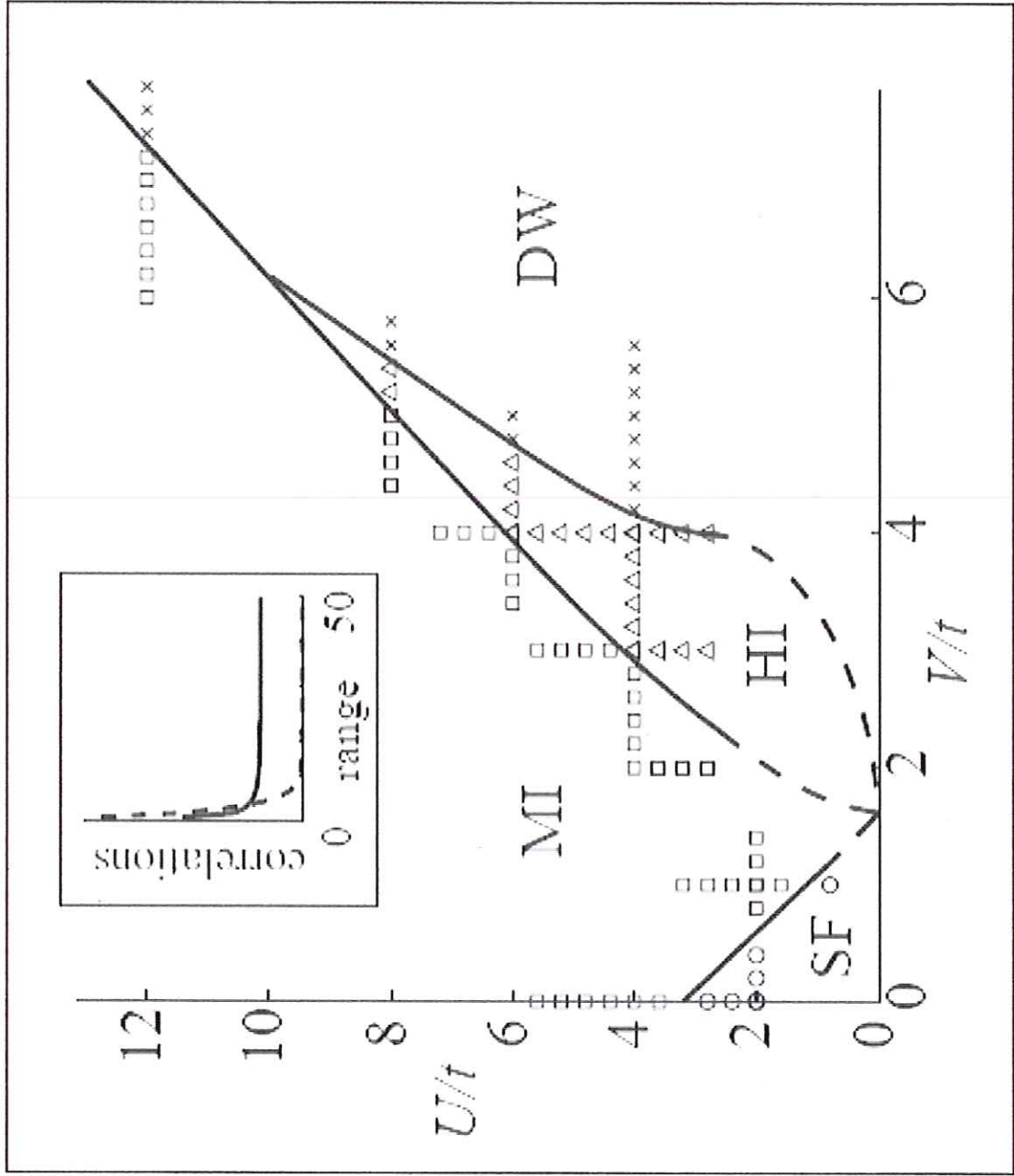
It's interesting that for growing dipolar interaction the funny goes from non-local (BCS-like) to local (i.e. one particle on top of the other)  $\xrightarrow{\text{dimer}} \text{BEC-like} \rightarrow \text{BCS-BEC crossover}$ .

(see p. 135).



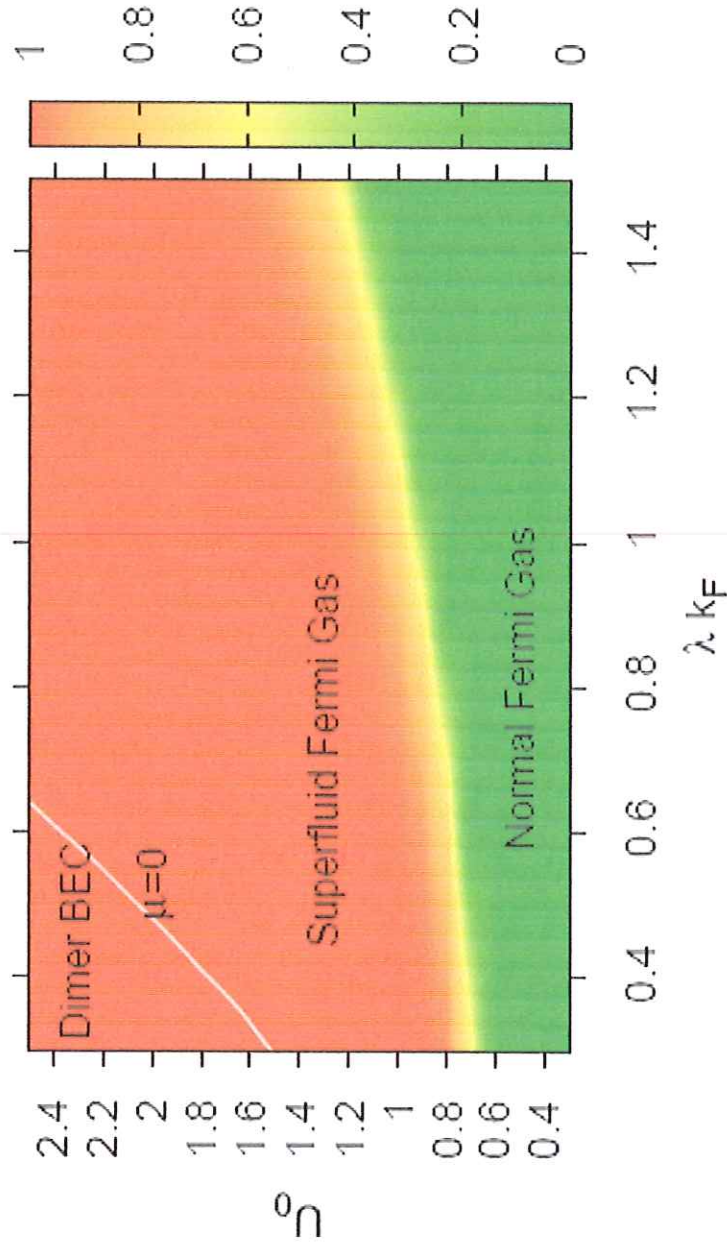
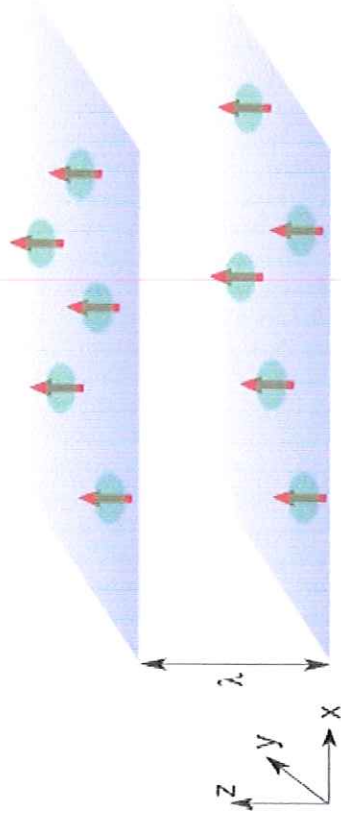
# Haldane insulator

[Dalla Torre et al. PRL  
97, 260401 (2006)]



# Inter-layer superfluidity

[Pikovsky et al., PRL 105, 215302 (2010)]



\* SPIN MODELS USING DIPOLE LATTICE GASES

\* Polar lattice gases open as well very attractive possibilities to study spin lattice models, as we will see from different perspectives.

\* let's consider first the extended Hubbard model up to nearest neighbor interactions for simplicity.

$$H = -t \sum_{\vec{j}, \vec{\delta}} [ b_{\vec{j}}^{\dagger} b_{\vec{j}+\vec{\delta}} + h.c. ] + \frac{U_0}{2} \sum_{\vec{j}} n_{\vec{j}} (n_{\vec{j}} - 1) + \frac{U_1}{2} \sum_{\vec{j}, \vec{\delta}} n_{\vec{j}} n_{\vec{j}+\vec{\delta}}$$

let's consider the hard-core case ( $U_0 \rightarrow \infty$ ) such that double-occupancy at any site is energetically very expensive. In that case we may safely assume  $(b_{\vec{j}}^{\dagger})^2 = 0$ , and hence  $n_{\vec{j}} = 0, 1$  in all sites.

We may then map the bosonic system into a spin-1/2 model,

by mapping occupation into spin:  $|n=0\rangle \Rightarrow |\uparrow\rangle$   
 $|n=1\rangle \Rightarrow |\downarrow\rangle$

More rigorously we introduce the spin-1/2 operators:  $\hat{S}_{\vec{j}}^{\pm} \equiv b_{\vec{j}}^{\dagger} ; \hat{S}_{\vec{j}}^z \equiv \frac{1}{2} - n_{\vec{j}}$

(Note: This is an example of a so-called Holstein-Primakoff transformation)

Then the tunneling part transforms into:

$$H_{\text{TUN}} = -t \sum_{\vec{j}} \sum_{\vec{\delta}} (b_{\vec{j}}^{\dagger} b_{\vec{j}+\vec{\delta}} + h.c.) = -t \sum_{\vec{j}, \vec{\delta}} (\hat{S}_{\vec{j}}^{-} \hat{S}_{\vec{j}+\vec{\delta}}^{+} + \hat{S}_{\vec{j}+\vec{\delta}}^{-} \hat{S}_{\vec{j}}^{+})$$
$$= -2t \sum_{\vec{j}, \vec{\delta}} (\hat{S}_{\vec{j}}^x \hat{S}_{\vec{j}+\vec{\delta}}^x + \hat{S}_{\vec{j}}^y \hat{S}_{\vec{j}+\vec{\delta}}^y)$$

The hopping term becomes a ferromagnetic (since  $-2t < 0$ ) XY spin Hamiltonian. That's all we would have without the dipole-dipole  $U_{\perp}$  term. [Note that lattice shelling may allow the change of sign(t) and hence one would have and Antiferro coupling as well.]

\* The  $U_1$  term becomes:

$$\frac{U_1}{2} \sum_{\vec{j}, \vec{\sigma}} n_{\vec{j}} n_{\vec{j}+\vec{\sigma}} = \frac{U_1}{2} \sum_{\vec{j}, \vec{\sigma}} \left( \frac{1}{2} - \hat{S}_{\vec{j}}^z \right) \left( \frac{1}{2} - \hat{S}_{\vec{j}+\vec{\sigma}}^z \right)$$

$$= \left( \frac{U_1}{8} \sum_{\vec{j}, \vec{\sigma}} \right) + \underbrace{\frac{U_1}{2} \sum_{\vec{j}, \vec{\sigma}} (\hat{S}_{\vec{j}}^z + \hat{S}_{\vec{j}+\vec{\sigma}}^z)}_{\text{This just regularizes the chemical potentials}} + \underbrace{\frac{U_1}{2} \sum_{\vec{j}, \vec{\sigma}} \hat{S}_{\vec{j}}^z \hat{S}_{\vec{j}+\vec{\sigma}}^z}_{\text{This is the truly relevant contribution}}$$

This is an irrelevant constant

[Note that  $-\mu \sum_{\vec{j}} n_{\vec{j}} \Rightarrow -\mu \sum_{\vec{j}} (\frac{1}{2} - \hat{S}_{\vec{j}}^z)$ ]

This is the truly relevant contribution

• Combining  $H_{\text{Hof}}$  and  $H_{\text{int}}$ , we obtain the final form of the spin Hamiltonian

$$\hat{H} = -2t \sum_{\vec{j}, \vec{\sigma}} (\hat{S}_{\vec{j}}^x \hat{S}_{\vec{j}+\vec{\sigma}}^x + \hat{S}_{\vec{j}}^y \hat{S}_{\vec{j}+\vec{\sigma}}^y) + \frac{U_1}{2} \sum_{\vec{j}, \vec{\sigma}} \hat{S}_{\vec{j}}^z \hat{S}_{\vec{j}+\vec{\sigma}}^z \quad J = -2t$$

$$\hat{H} = J \sum_{\vec{j}, \vec{\sigma}} \left( \hat{S}_{\vec{j}}^x \hat{S}_{\vec{j}+\vec{\sigma}}^x + \hat{S}_{\vec{j}}^y \hat{S}_{\vec{j}+\vec{\sigma}}^y + \frac{U_1}{2J} \hat{S}_{\vec{j}}^z \hat{S}_{\vec{j}+\vec{\sigma}}^z \right)$$

↳ XXZ Heisenberg model

For the particular case of  $U_1/2J = 1$  we recover the isotropic Heisenberg Hamiltonian we discussed in p. 31 in the context of superexchange.

\* Note, however, that whereas the superexchange scale was  $t^2/U$ , here the spin-spin interaction is given by the hopping,  $t$ , (for the  $xy$  interactions) and the inter-site dipole-dipole interaction,  $U_1$ , for the  $zz$  interactions. These scales may be much larger than  $t^2/U$ , and hence spin modes with dipolar gases may be easier to study.

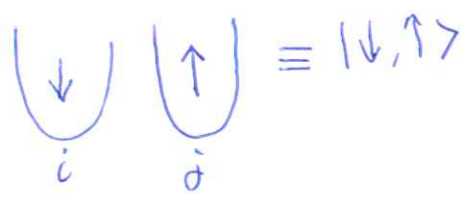
\* A second relevant point is that dipolar interactions may lead to relevant interactions between spins placed far apart, which is not possible with superexchange.

\* Using the rotational degree of freedom as a spin in polar molecules in optical lattices

In our discussion of p. (123) we discussed about the rotational states, and in particular about the necessity of admixing rotational states to "activate" the dipole-dipole interaction.

As mentioned in p. (124) even in the absence of a d.c. electric field, dipolar interactions can be established using a microwave field to create a coherent superposition between two rotational states (see p. (142)). This two states will act like a pseudo-spin-1/2, and we will hence call them  $|\uparrow\rangle$  and  $|\downarrow\rangle$ .

Let's consider two molecules, one at site  $i$  and the other at site  $j$ . Let's consider that one molecule is in the state  $|J=0, M=0\rangle = |\downarrow\rangle$  and the other is in  $|J=1, M=-1\rangle = |\uparrow\rangle$ .



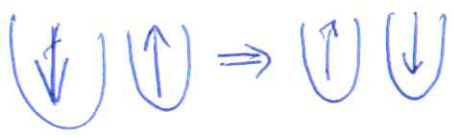
The two molecules interact via the dipole-dipole interaction: 
$$H_{DDi} = \frac{1}{4\pi\epsilon_0 r^3} \left[ \vec{d}_1 \cdot \vec{d}_2 - 3 \frac{(\vec{d}_1 \cdot \vec{r})(\vec{d}_2 \cdot \vec{r})}{r^2} \right]$$

where  $\vec{r} = (\vec{r}_i - \vec{r}_j)$

As we already mentioned in p. (124):  $\langle J=0, M=0 | \hat{d} | J=0, M=0 \rangle = 0$  and  $\langle J=1, M=-1 | \hat{d} | J=1, M=-1 \rangle = 0$  (this is true for any  $(J, M)$ ). [This is because  $\hat{d} \sim Y_{1m}$ , and hence the Clebsch-Gordan coefficients are zero]. However  $\langle 0,0 | \hat{d} | 1,-1 \rangle = d/\sqrt{3}$  (where  $1/\sqrt{3}$  is the Clebsch-Gordan coefficient).

As a result one has a non-zero matrix element  $\langle \uparrow \downarrow | H_{DDi} | \downarrow \uparrow \rangle$

$$\rightarrow \frac{1}{3} \left( \frac{d^2}{4\pi\epsilon_0 r^3} \right) (1 - 3\cos^2\theta)$$



One can hence a dipole-induced spin flip-flop

\* Hence, in the absence of an applied electric field, two-level polar molecules trapped in a strong 3D lattice can be described using a spin-1/2 lattice model:

$$\hat{H} = \frac{J_{\perp}}{2} \sum_{\langle i,j \rangle} V_{dd}(\vec{r}_i - \vec{r}_j) (S_i^+ S_j^- + S_i^- S_j^+)$$

$\theta$  is the angle between  $\vec{r}$  and the quantization axis.

with  $J_{\perp} = \frac{-d^2/3}{4\pi\epsilon_0}$  and  $V_{dd}(\vec{r}) = \frac{1}{r^3} (1 - 3\cos^2\theta)$

(see below)

\* Hence the dipolar interactions lead to an effective XY Hamiltonian, but now the interaction doesn't limit to nearest neighbors, and it's in addition anisotropic (see p. 142).

\* These effective flip-flops were recently studied at JILA in KRb molecules in 3D lattices [B. Yan et al., Nature 501, 521 (2013)]. In these experiments the lattice is  $\mu\text{m}$  large ( $\sim 40 E_{\text{rec}}$ ) that one can forget the molecular hopping.

They employ microwaves to couple  $|0,0\rangle$  and  $|1,-1\rangle$ . The degeneracy of the rotational levels is broken by the interaction between the nuclear quadrupole moments and the rotation of the molecules. Using a magnetic field the states  $|1,0\rangle$  and  $|1,+1\rangle$  are pushed out of resonance (for  $B = 546 \text{ G}$ ,  $|1,0\rangle$  and  $|1,+1\rangle$  are pushed 270 and 70 kHz, respectively). The quantization axis mentioned above is then set by the magnetic field, which is oriented at  $45^\circ$  with respect to the x and y directions (see p. 142).

The polarization of the lattice beams is chosen such that the lattice is basically identical for  $|1,\downarrow\rangle$  and  $|1,\uparrow\rangle$ .

Following the arguments mentioned above, each molecule in the lattice will experience an interaction energy with contributions from all other molecules (depending on their mutual distance and relative angle).

\* let's discuss briefly how the existence of these inter-site spin flip-flops was revealed in experiments by means of coherent microwave spectroscopy (see p. 142).

Starting with all molecules in  $|↓⟩$ , a  $\frac{\pi}{2}$  pulse created a superposition  $(|↓⟩ + |↑⟩)/\sqrt{2}$ . After a free evolution time  $T/2$ , a pulse  $\pi$  was applied, followed by another free-evolution time  $T/2$  and a final  $\pi/2$  pulse.

[Note that the  $\pi$  pulse acts as a so-called echo pulse. Any residual ac Stark shift that leads to single-particle dephasing is removed using the echo technique (the spins dephase and then rephase after the echo.)]

At the end the number of  $|↓⟩$  molecules is measured as a function of the phase offset of the last  $\pi/2$  pulse with respect to the initial  $\frac{\pi}{2}$  pulse. This yields a Ramsey fringe (see p. 143).

In absence of interactions between the spins, and since one employs the echo technique, one would expect a maximal and constant contrast of the Ramsey fringes. Hence measuring the evolution of the contrast in time yields information on spin-spin interactions (Note: flip-flops obviously scramble the spin evolution, and hence the Ramsey interferometer.)

In the contrast curves one sees (p. 143):

- \* Oscillations.
- \* Overall decay
- \* Imperfect lattice filling (which is not fully known but should be about 10%) and spin-spin interactions give a spread of interaction energies that results in dephasing, and hence decaying, contrast. (see p. 143)
- \* For low fillings (as it is the case) the interaction energy spectrum can have a strong contribution from the highest-magnitude nearest-neighbor interaction. The beating of this frequency with the contribution from molecules that experience negligible shifts justifies the observed oscillations.

\* A simple calculation shows that the maximal interaction to nearest neighbors in JILA's experiment is  $\sim 52$  Hz. The observed oscillation is  $\sim 48 \pm 2$  Hz in good agreement.

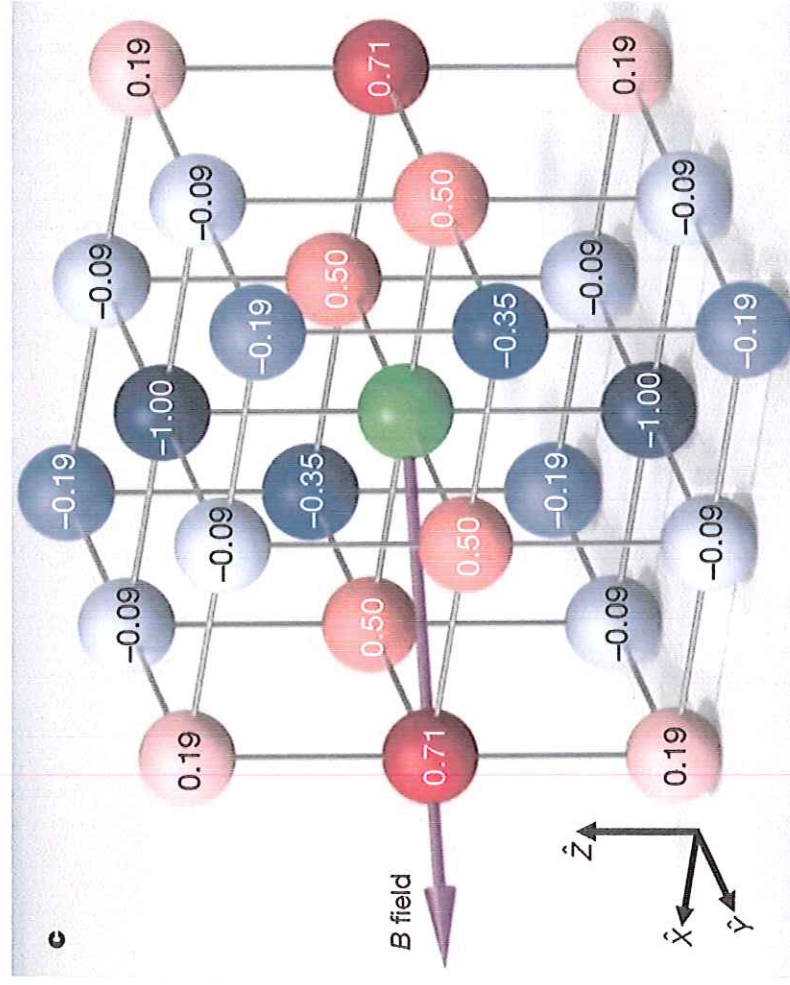
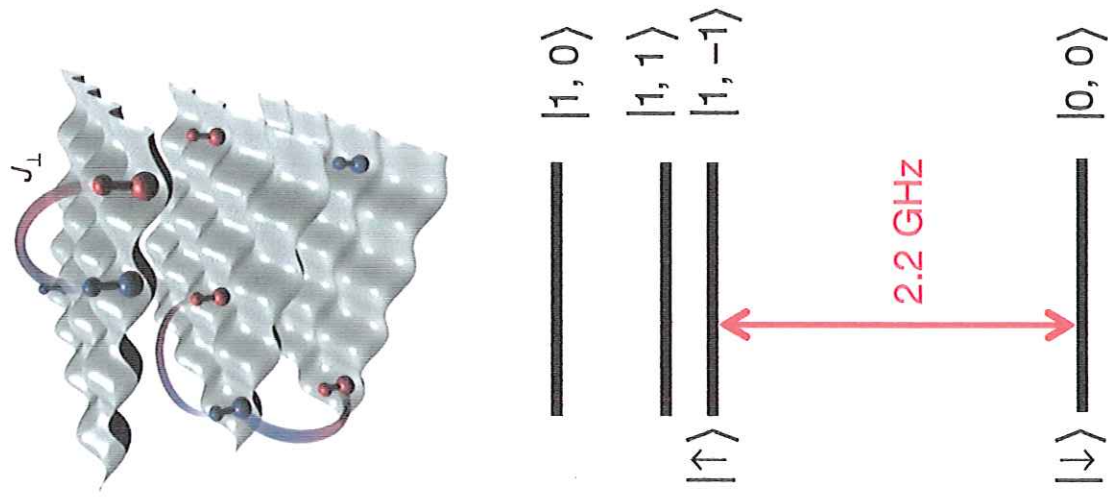
\* They also observe that the larger the filthy the ~~slower~~ faster the contrast damping (see p. 143) as one would expect, since there's a growing probability that molecules have multiple neighbors, and more spin-exchange frequencies contribute to the signal, enhancing the dephasing

\* This experiments have shown convincingly the existence of pairwise spin exchange induced by dipolar interactions in polar molecules in optical lattices, and open interesting possibilities that I will discuss later on.



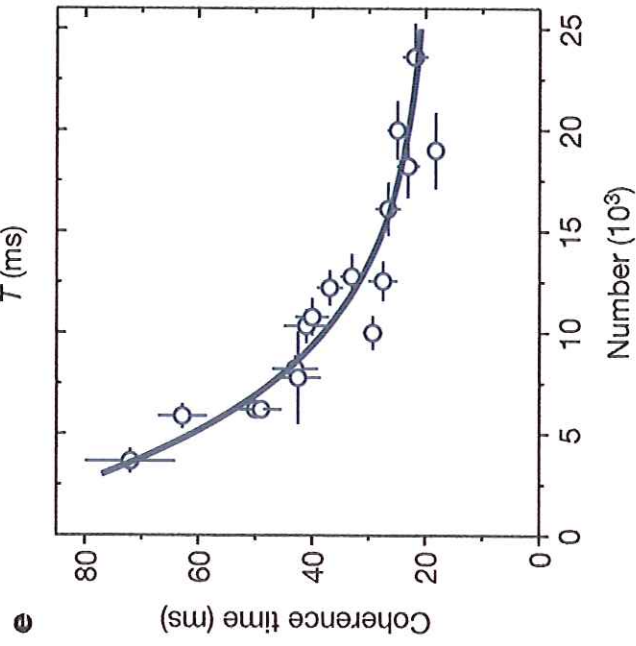
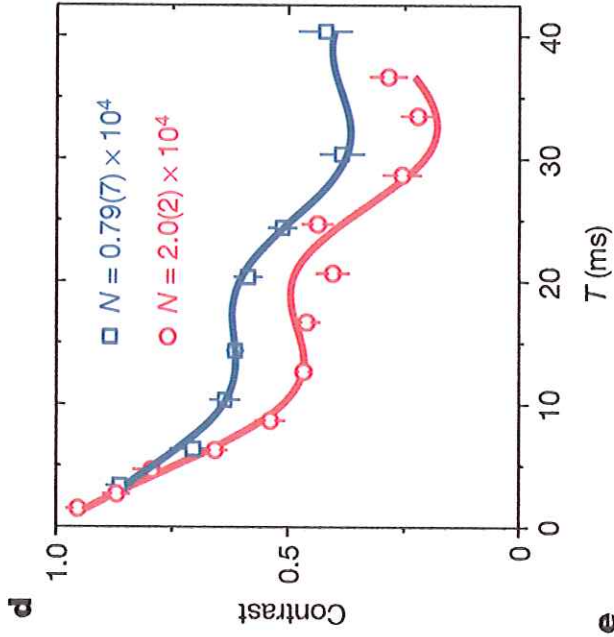
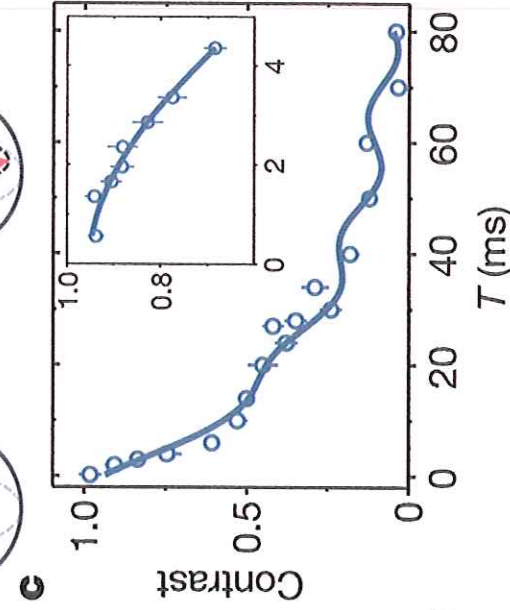
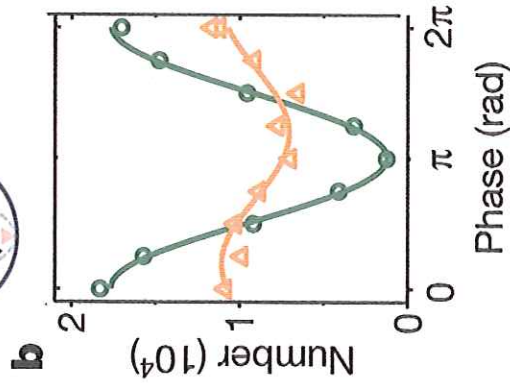
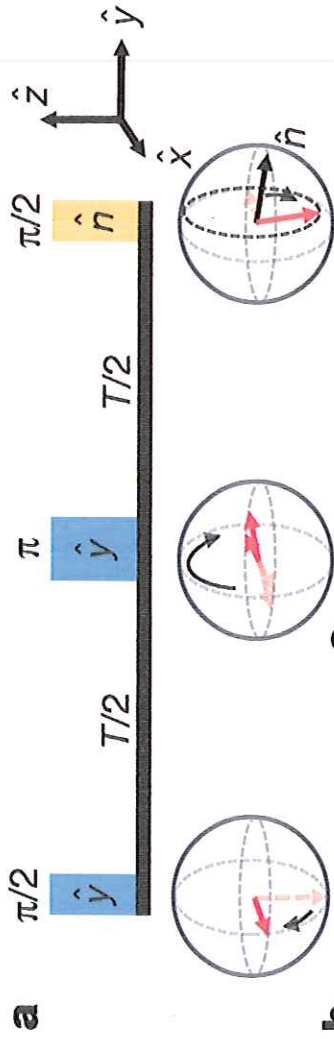
# Dipole-induced spin exchange in polar molecules

[Yan et al., Nature 501, 521 (2013)]



# Dipole-induced spin exchange in polar molecules

[Yan et al., Nature 501, 521 (2013)]



\* Quantum magnetism in a dipolar lattice gas formed by chromium atoms

\* The effects of intersite spin-spin interactions were studied as well in lattice gases formed by magnetic atoms in a recent experiment performed (using  $^{52}\text{Cr}$  atoms) at B. Laburthe's lab in Paris Nord.

\* Before moving to this experiment we should recall a couple of important issues concerning spinor gases, i.e. gases of atoms with more than 2 internal levels.

\* Chromium is a peculiar spinor gas, since it presents spin  $S=3$  (no hyperfine structure in Cr). It has then  $M_S = -3, \dots, 3 \Rightarrow$  seven possible internal components.

\* Let's have first a look to the short-range interactions. When 2 particles interact, their spins couple to form a total spin during the collision. Recall that for two particles of spin  $S$ , the total spin ranges from  $S_T = 0$  to  $2S$  (every  $\pm 1$ ). Recall that bosons must keep symmetric both in spin and motional degree of freedom. This means that the spin part must keep symmetric to collide in s-wave  $\rightarrow$  hence  $S_T = 0, 2, \dots, 2S$  even.

\* Associated to each available  $S_T$  there's an s-wave scattering length:  $a_{S_T}$ , such that the interaction Hamiltonian is of the form:

$$\hat{H}_{INT} = \frac{1}{2} \sum_{S_T} g_{S_T} \hat{P}_{S_T}$$

with  $g_{S_T} = 4\pi\hbar^2 a_{S_T} / m$  and  $\hat{P}_{S_T}$ : projector operator onto a 2-particle state with total spin  $S_T$ .

\* Short-range collisions preserve the spin projection along the quantization axis. [Note: This is most surely not the case in species like Dy or Er that present anisotropic short-range interactions, but how the scattering is remains at the moment unclear; for Cr the situation is simpler due to isotropy].

This means that if we collide 2 particles with spin projections  $m_1$  and  $m_2$ , after the collision we will have  $m_3$  and  $m_4$ , such that  $m_1 + m_2 = m_3 + m_4$ .

Note that this may be done in 2 non-equivalent ways  
either  $\left\{ \begin{matrix} m_1 = m_3 \\ m_2 = m_4 \end{matrix} \right.$  or  $\left\{ \begin{matrix} m_1 = m_4 \\ m_2 = m_3 \end{matrix} \right.$  or  $m_{1,2} \neq m_{3,4}$ . The latter

possibility leads to the so-called spin-changing collisions.

One may show that these collisions result from the differences between the scattering lengths  $a_{ST}$ .

[Note: for alkali-earth fermions of fermionic  $Yb$ , the lowest manifold presents the same scattering length for all collisions, and hence spin-changing collisions are forbidden, leading to SU(N) systems.]

\* Spin-changing collisions play a crucial role in the physics of spinor gases, since they lead to spinor dynamics, i.e to a transfer between different spin components.

\* let's have a look now to the role of dipole-dipole interactions.  
The dipole-dipole interaction between two <sup>magnetic</sup> atoms having

spin  $\vec{S}$  is:  
$$A_d = \frac{\mu_0 \hbar^2}{4\pi m_e r^3} \left[ \vec{S}_1 \cdot \vec{S}_2 - 3(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r})/r^2 \right]$$

The dipole-dipole interaction leads as well to spin-changing collisions as those discussed above. It leads in principle to something else. Note that the dipole-dipole interaction is anisotropic (in the language of spherical harmonics it contains  $Y_{2m}$  terms). As a result it may induce a transfer of orbital angular momentum, which if symmetry is altered, should be compensated by a corresponding change in the spin projection of the colliding pair. This effect

(similar to the celebrated Einstein-de Haas effect) leads to spin relaxation. This effect may be interesting for several reasons (including demagnetization cooling) but for our purposes here it's rather something to avoid. This may be easily done by properly choosing the amplitude of the orienting magnetic field (note that since spin relaxation changes the spin projection it's characterized by a Zeeman energy shift).

• The 2-particle <sup>dimer</sup> Hamiltonian hence reduces to

$$H_d = \frac{J_0 \mu^2}{4\pi r^3} \left(1 - 3 \frac{z^2}{r^2}\right) \left[ \hat{S}_1^z \hat{S}_2^z - \frac{1}{4} (\hat{S}_1^+ \hat{S}_1^- + \hat{S}_1^- \hat{S}_1^+) \right]$$

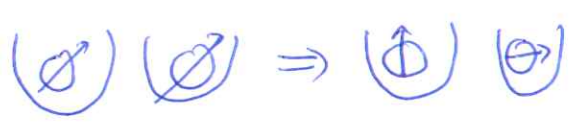
One gets hence an XXZ Hamiltonian. Note that here we have both :: spin exchange terms:  $S^+ S^-$

• Ising-like terms:  $S^z S^z$

Note also that we are not dealing here with spin-1/2 particles but rather with a spin-3 system.

\* If we place the particles such that there's only one particle per site then we ~~recover a~~ obtain a spin-3 Heisenberg XXZ Hamiltonian.

Intersite spin-spin interactions lead to spin-changing collisions even for singly-occupied sites.



Note that this would be excluded if we only had onsite interactions.

\* For the experiments in Paris Nord, they prepare a Mott state of particles in  $M_s = -3$ . They blow up doubly (or hybrid) occupied sites and hence there are just ~~single occupied sites~~ <sup>singly occupied sites</sup> and holes.

\* Under the conditions of the experiment they have a wide shell of single occupied sites with very few holes. The lattice is very deep forbidding (to a large extent) mobility. ~~As a result~~

\* In a second stage atoms are transferred to  $m_s = -2$ . Note that:  $(-2) (-2) \Rightarrow (-3) (-1)$  is possible now due to inter-site spin-doubling collisions. As a result the ~~spin~~ populations of the different components evolve in time (they would be completely frozen ~~in~~ in absence of inter-site interactions) (see p. 149)

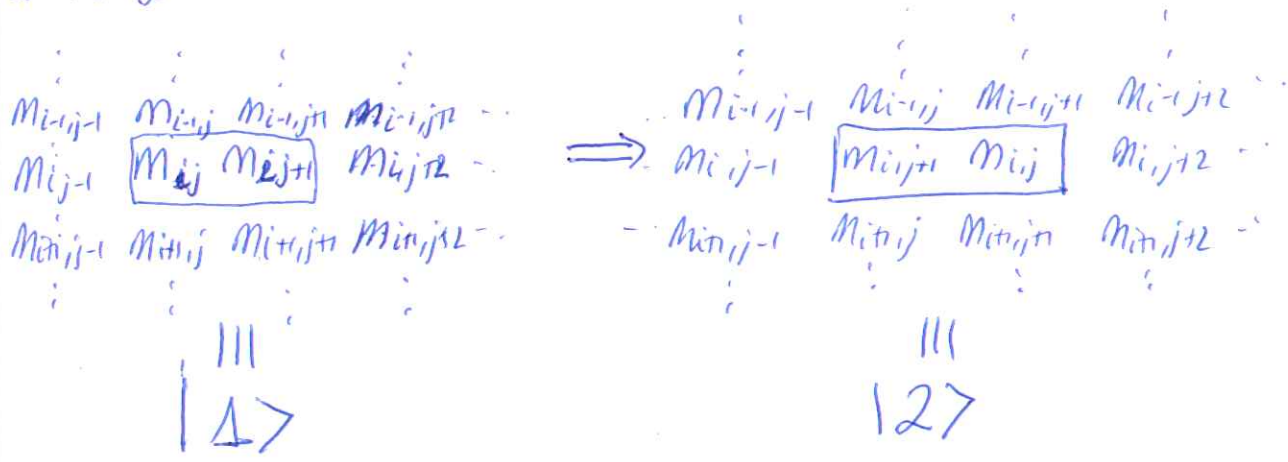
\* The existence of spin dynamics is already a clear proof of the inter-site spin-spin interactions. Moreover the dynamics is nicely covered by an effective Hamiltonian:

$$\hat{H} = - \sum_{\langle ij \rangle, m_s} J_{ij} b_{i, m_s}^{\dagger} b_{j, m_s} + g \sum_{j, m_s} m_s^2 \hat{n}_{j, m_s} + \sum_{ij} V_{ij} (S_i^z S_j^z - \frac{1}{4} (S_i^+ S_j^- + S_i^- S_j^+))$$

hopping of holes (actually not so relevant)  
 residual quadratic ~~energy~~  
~~effect~~ light shift  
 inter-site spin-spin interactions.

\* One can see that the dynamics of the spin is well described by this model (p. 149).

\* An interesting point to note here is that the dynamics is inherently many-body. In particular mean-field theories do a rather poor job. That's rather easy to grasp. Let's consider two spin configurations which ~~can~~ be connected by a spin-exchange:

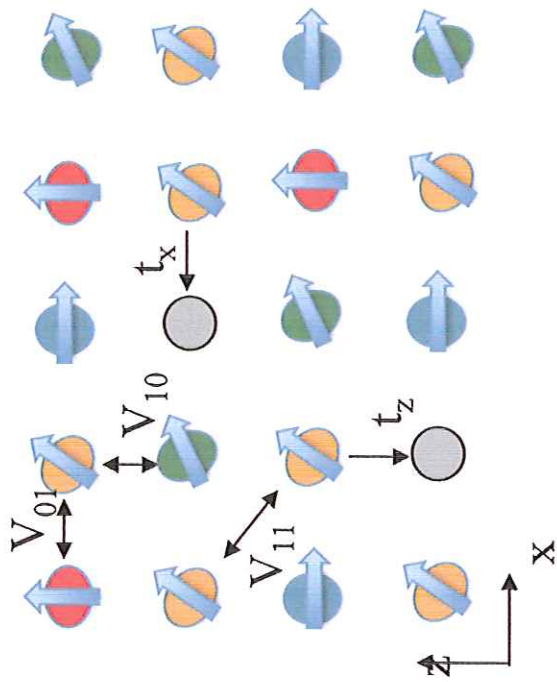
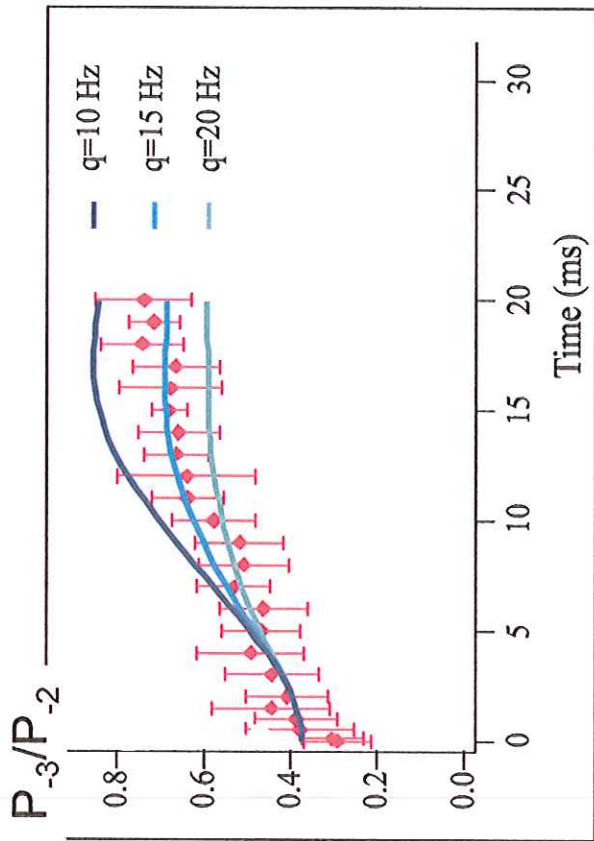
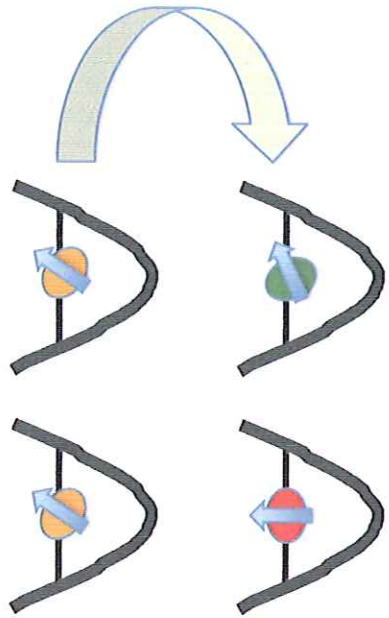
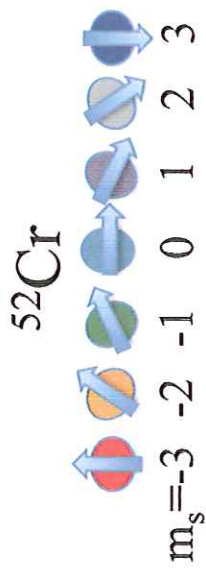


\* If we call these two many-body states  $|1\rangle$  and  $|2\rangle$  then we see that due to the  $S^2 S^2$  term, the energy difference of  $|1\rangle$  and  $|2\rangle$ ,  $\Delta E = E_1 - E_2$ , is determined by the <sup>particular</sup> spin configuration of the neighbors. If  $\Delta E \gg$  coupling energy between  $|1\rangle$  and  $|2\rangle$  given by the spin-exchange, then the spin-exchange is prevented since it's far from resonance.

\* Mean-field theories <sup>(at least simple ones)</sup> will not recover this effect, since they will consider a mean effect of the spins. If  $\langle m_{ij} \rangle$  is uniform then both  $E_1 = E_2$ , and hence exchange is always resonant. However we just saw that fluctuations may crucially drive  $\Delta E \gg$  coupling. As a result the actual many-body dynamics is significantly slower than the mean-field one!

# Quantum magnetism in a Cr lattice gas

[De Paz et al., PRL 111, 185305 (2013)]





\* Modifying the effective spin interaction between polar molecules

\* Using a combination of dc electric field and microwave dressing one may get a rich variety of possibilities for spin-spin interactions, which we will briefly discuss here in a simplified way [for a throughout discussion see e.g. Micheli et al., Nature Physics 2, 341 (2006), and Garshkov et al., PRA 84, 033619 (2011)].

\* We ignore the nuclear degree of freedom, assume negligible tunneling, and consider the simplest scenario of a single molecule per site. One gets the Hamiltonian we mentioned above (but with  $s^z s^z$  terms)

$$H = \frac{1}{2} \sum_{i \neq j} V_{dd}(\vec{R}_i - \vec{R}_j) \left[ J_z s_i^z s_j^z + \frac{J_+}{2} (s_i^+ s_j^- + s_i^- s_j^+) \right]$$

- \* The interaction may be tuned by:
  - \* changing the magnitude and orientation of the dc field
  - \* choosing different rotational states as the pseudospin-1/2
  - \* Modifying the number, frequency and intensity of the applied microwaves.

\* The first 2 points should be rather clear from previous discussions. So let's have a look to the microwave issue.

As in the discussion of p. (123), the rotational physics (+ effect of the dc field) is given by:

$$H_0 = B J^2 - d_0 E$$

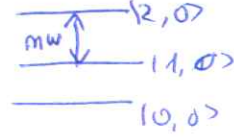
The microwave introduces a second term:

$$H_{mw} = -\vec{d} \cdot (E_{mw} \vec{e}_{mw} e^{i\omega_{mw}t} + c.c.)$$

In addition, between 2 molecules we will have the dipolar interaction.

\* By playing with the dc field and the mw frequency we may resonantly couple 2 rotational states. We may for example couple  $|1,0\rangle$  and  $|2,0\rangle$  using a linearly polarized microwave:  $|m_1\rangle \equiv \sqrt{a} |1\rangle + \sqrt{1-a} |2\rangle$  (there is of course a second dressed state but we will consider only this one for our pseudospin-1/2). As the other pseudospin-1/2 we

choose  $|m_0\rangle \equiv |0,0\rangle$ .



We may evaluate the dipole terms:

$\langle m_0 | d | m_0 \rangle = 0$  in absence of dc field  
 (but it's non zero if  $|0,0\rangle \rightarrow |\phi_0\rangle$  the eigenstate of  $B_0^2 - d_0 E$ )

$\langle m_1 | d | m_1 \rangle = 2\sqrt{a(1-a)} \underbrace{\langle 10 | d | 20 \rangle}_{\mu_{12}} \rightarrow J_z = 4a(1-a)\mu_{12}^2$

$\langle m_0 | d | m_1 \rangle = \sqrt{a} \underbrace{\langle 00 | d | 10 \rangle}_{\mu_{01}} \rightarrow J_\perp = 2a\mu_{01}^2$

One can hence control the ratio  $J_z/J_\perp$  with the dressing  $a$ .

Playing with microwave dressings and dc fields one may engineer quite exotic families of lattice Hamiltonians of the general form:

$H \propto \sum_{\alpha,\beta=0}^3 \sigma_i^\alpha A_{\alpha\beta}(\vec{r}) \sigma_j^\beta$  with  $\sigma^0 = \mathbb{1}$ ,  $\sigma^{1,2,3} = \sigma^{x,y,z}$

A possible example is a lattice like that of p. 152, where:

$H_{\text{spin}} = J_\perp \sum_{x \text{ links}} \sigma_j^x \sigma_k^x + J_\perp \sum_{y \text{ links}} \sigma_j^y \sigma_k^y + J_z \sum_{z \text{ links}} \sigma_j^z \sigma_k^z$

This is the so-called Kitaev model. By adjusting  $|J_\perp/J_z|$  the system may be tuned from a gapped phase carrying Abelian anyonic excitations to a gapless phase that, in the presence of a magnetic field, becomes gapped with non-Abelian excitations.

\*As a final comment, let me mention that if one considers all "spins" down and one flips one of them  $|\uparrow\rangle$ , then this excitation behaves as a boson  $\rightarrow$  recall the Holstein-Primakoff transformation of p. 136. As a result, a dilute gas of spin excitations (magnons) behaves as a Bose gas, which may Bose condense [see eg. Kwasigroch and Cooper, PRA 90, 021605(Q) (2014)].

# Modifying the spin interactions using mw dressing

[Micheli et al., Nature Phys. 2, 341 (2006);  
Gorshkov et al, PRA 84, 033619 (2011)]

