Polar molecules in optical lattices

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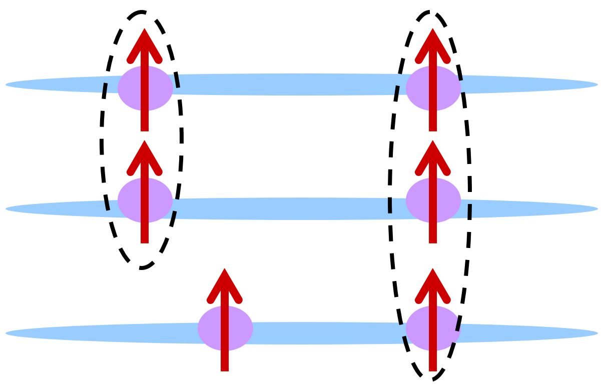
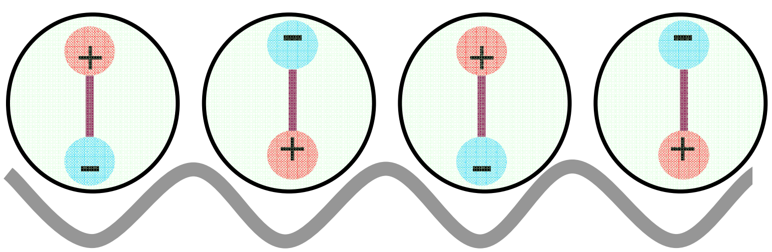
1) Chaining of polar molecules in a 1d optical lattice



Self-assembly into chains

Effects of chaining on BE condensation

2) Quantum magnetism with polar molecules in an optical lattice



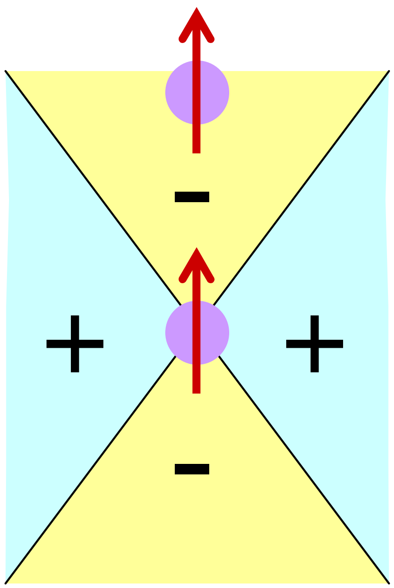
Long range spin interaction between
polar molecues by exchange of
a quantum of rotation

Spin ordering in Mott phases

Melting Mott phases

Self assembly of chains of polar molecules
or
Quantum rheological electrofluids of polar molecules
or
3D polar BEC without collapse

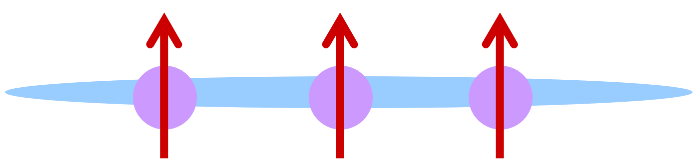
Results obtained by Charles Wang



Attractive part of dipolar interactions
can lead to collapse of
a 3D condensate

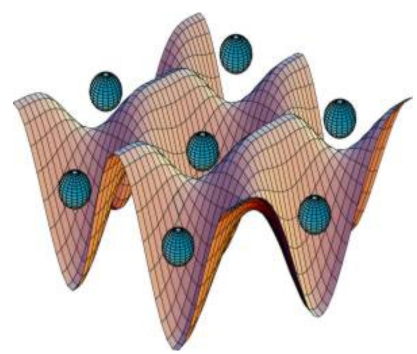
How to avoid collapse

Confine polar molecules in 2D



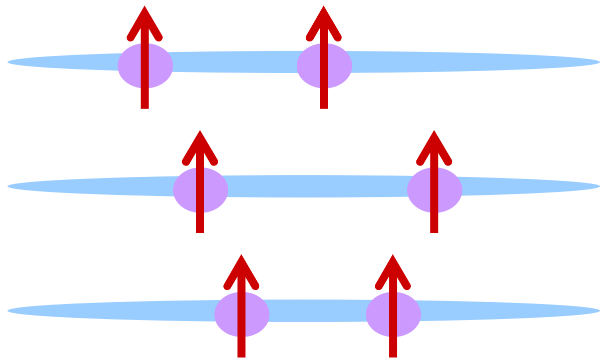
See e.g. Santos et al.

Polar molecules in optical lattices

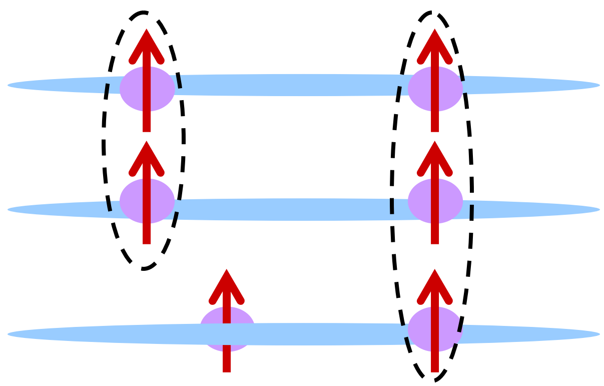


See e.g. Goral et al., Zoller et al.

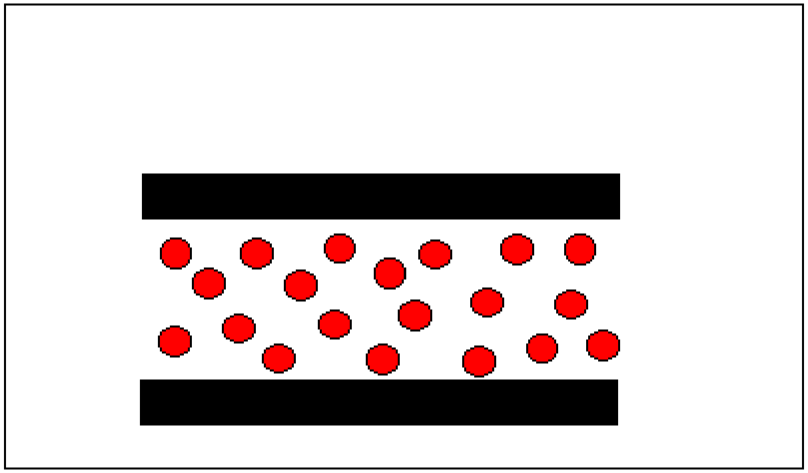
Polar molecules in an optical lattice of pancakes



Attraction between dipoles can lead to formation of bound states but not collapse

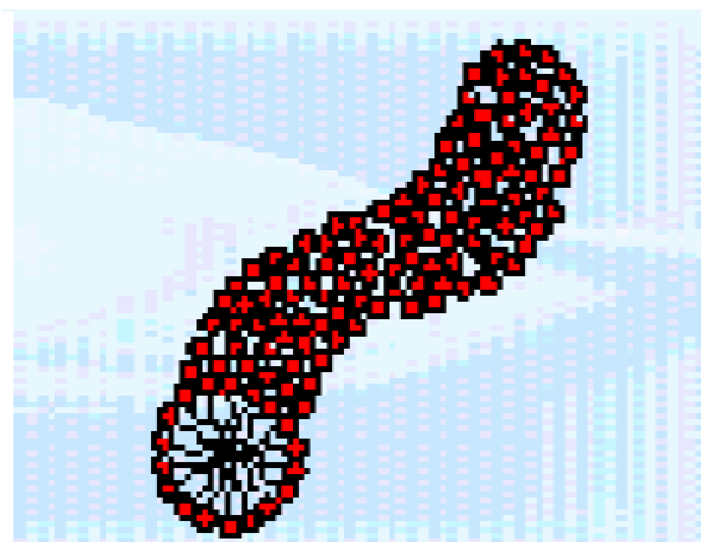


Chaining: self-assembly of particles into semiflexible chains



Ferrofluids:
nanoscale magnetic particles suspended in a carrier fluid.

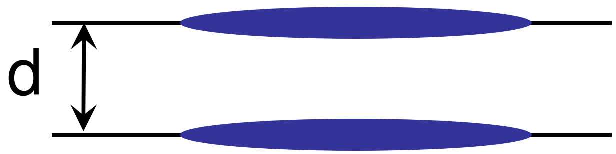
Electrofluids:
nanoscale dielectric particles suspended in a dielectric base fluid



Elongated micelles:
linear structures of amphiphilic molecules

Interlayer bound states of dipoles

Bilayer system



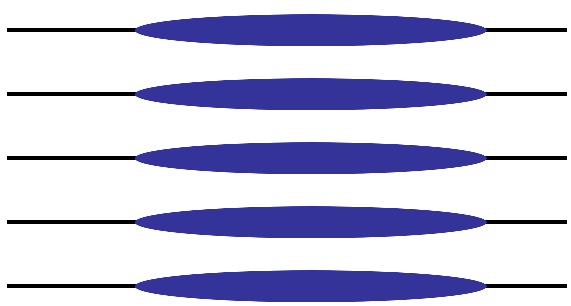
Bound state appears when interaction energy becomes comparable to kinetic energy

$$\frac{D^2}{d^3} \sim \frac{\hbar^2}{md^2}$$

Variational calculation with $\psi(r_1, r_2) = \frac{1}{\sqrt{\pi}R} e^{-\frac{(r_1 - r_2)^2}{2R^2}}$

Bound state appears when $\frac{D^2 m}{\hbar^2 d} = 1.6$

Infinite chain. Variational wavefunction $\psi(\{r_i\}) = \prod_i \frac{1}{\sqrt{\pi}R} e^{-r_i^2/2R^2}$

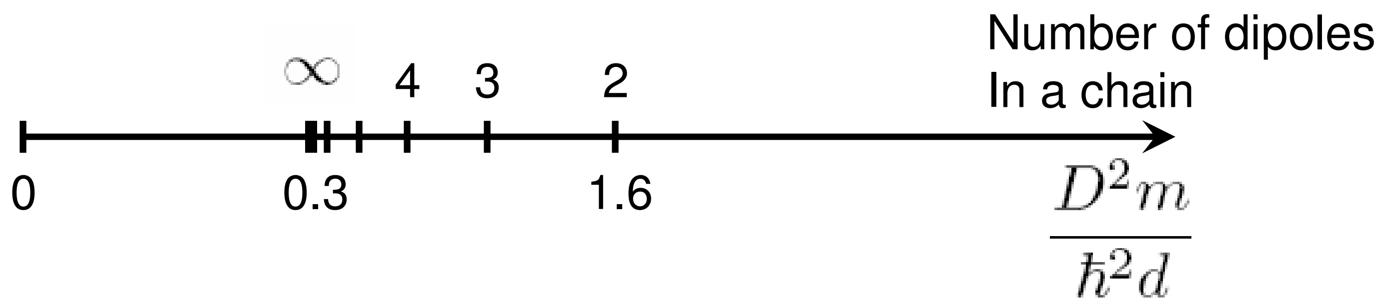


Bound state appears when

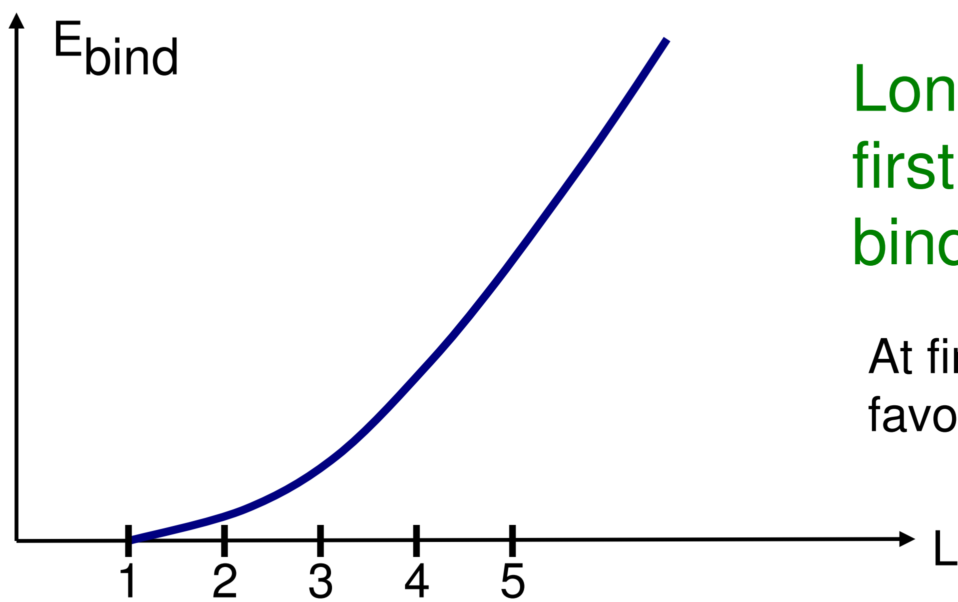
$$\frac{D^2 m}{\hbar^2 d} = 0.3$$

Interlayer bound states of dipoles

The order of appearance of bound states



Binding energy as a function of chain length

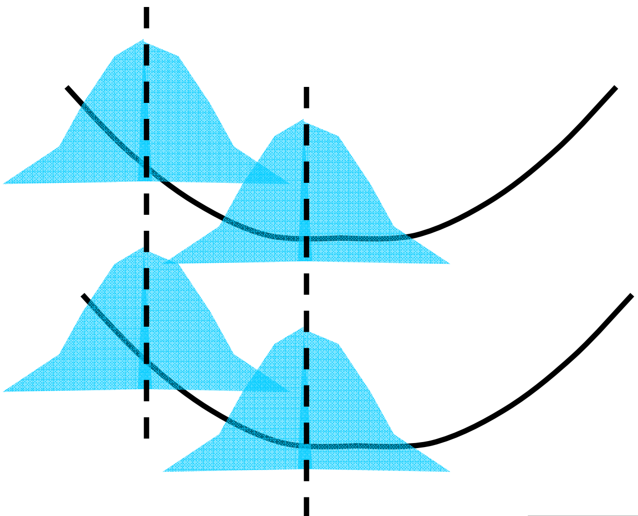


Longer chains appear first and have larger binding energies

At finite temperature entropy favors shorter chains

Chains of polar molecules. Thermodynamics

Neglect interactions between chains compared to in-plane parabolic potential



$$N\,\frac{D^2}{a_0^3} < \frac{\hbar^2}{m\,a_0^2}$$

a_0 in plane oscillator length

N number of molecules per layer

Together with $\frac{D^2 m}{\hbar^2 d} \sim 1$ this implies

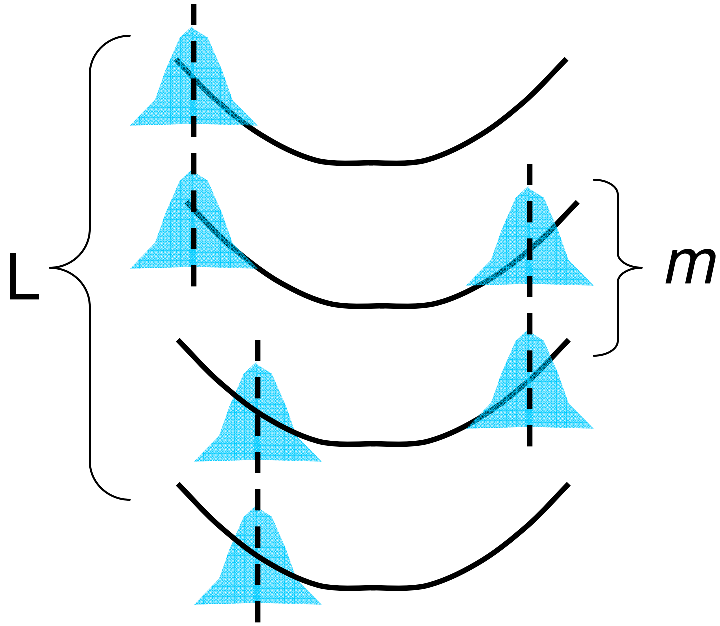
$$\boxed{N^2\,\hbar\omega_0 < E_R}$$

ω_0 in plane oscillator frequency

$E_R = \frac{\hbar^2}{m\,d^2}$ recoil energy of the optical lattice

Neglect bending of chains $\boxed{T < E_{bind}}$

Thermodynamics of non-interacting chains



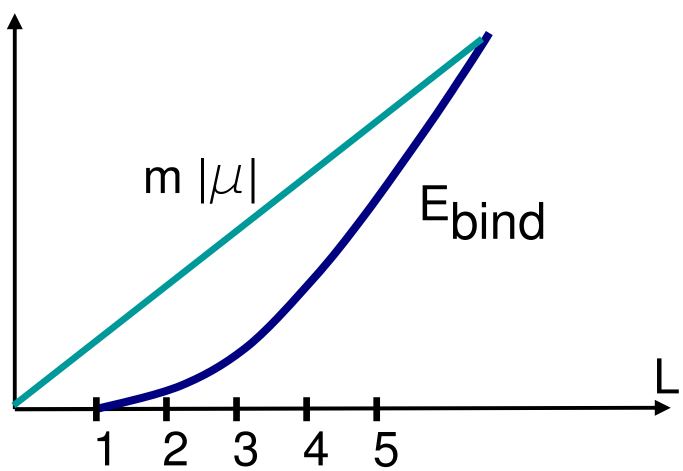
Chain of length *m* is characterized by:
in-plane quantum numbers (i_x, i_y)
and the vertical position

$$\epsilon_{m,i} = \hbar\omega_0(i_x + i_y + 1) - E_{bind}(m)$$

Number of chains of length *m*

$$N(m) = (L - m + 1) \sum_{i_x, i_y} \frac{1}{e^{\beta(\epsilon_{m,i} - m\mu)} - 1}$$

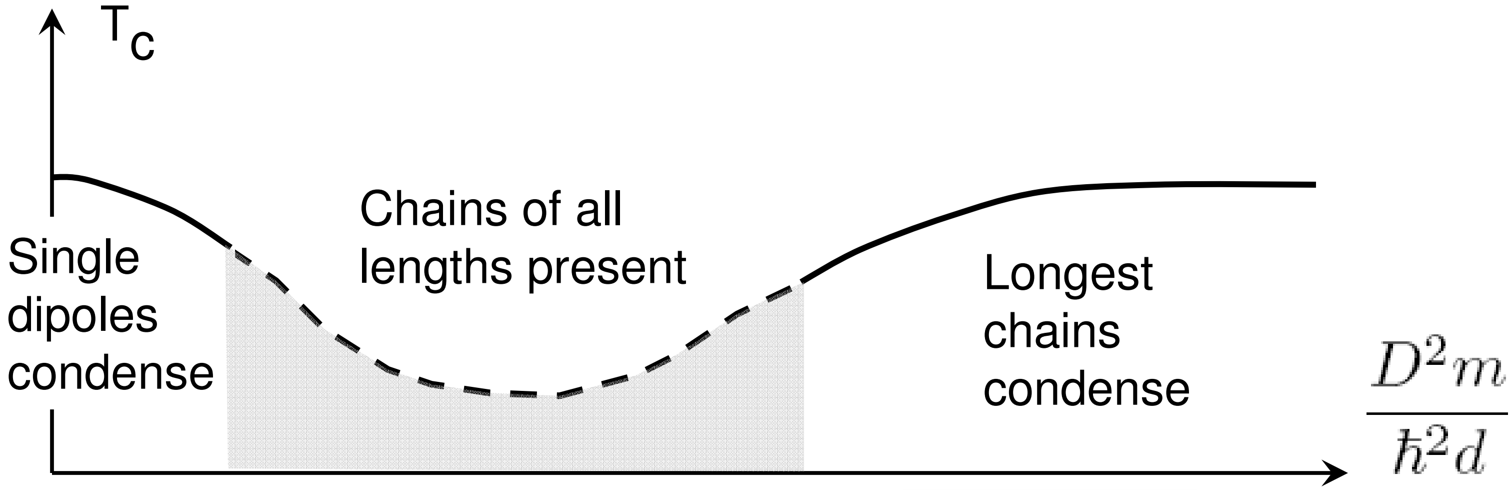
Condensation occurs when $\epsilon_{m,i} - m\mu = 0$



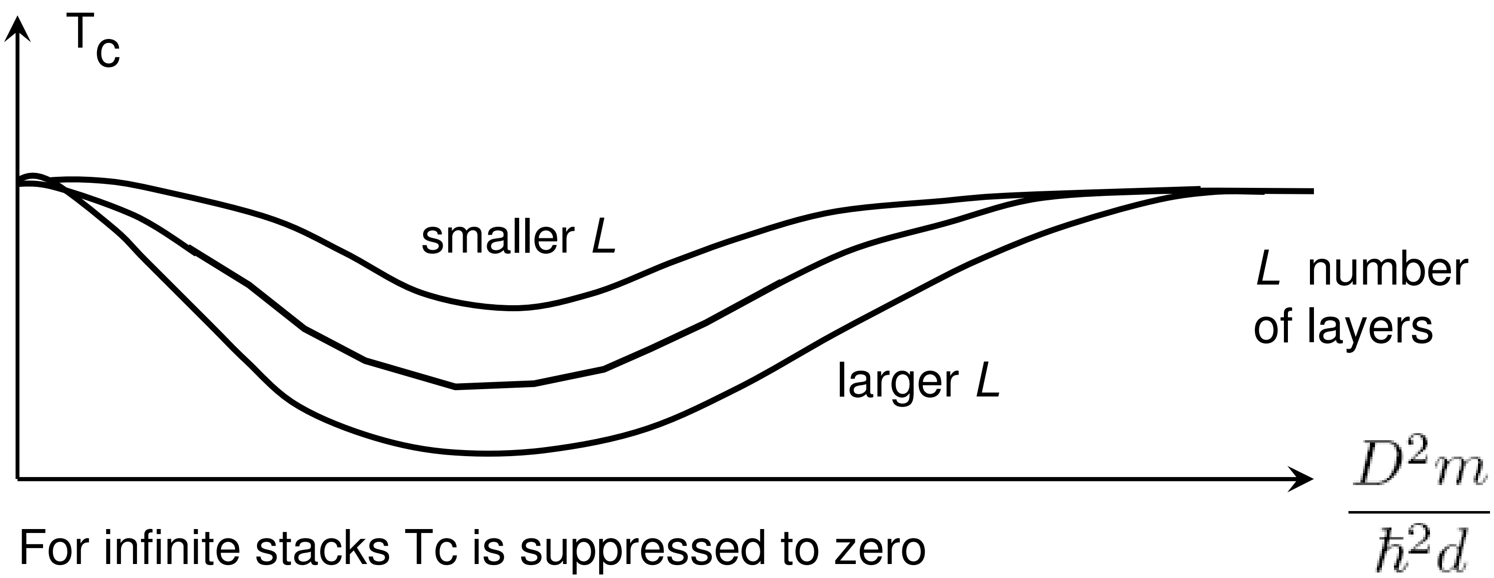
When ω_0 is small compared to E_{bind}

The longest chains condense first

Chains of polar molecules. Phase diagram



Suppression of Tc for smaller values of $D^2 m/\hbar^2 d$ comes from distributing dipoles over many types of chains



For infinite stacks Tc is suppressed to zero

Chaining of polar molecules in a 1d lattices

Chains will be formed when dipolar moments of molecules exceed a certain critical value. Longest chains are formed first and have the highest binding energy.

Distribution of chains is determined by the competition of entropy and binding energy. Chaining should play an important role in thermodynamics of polar molecules in 1d lattices even at high tempearatures

Longest chains BE condense first

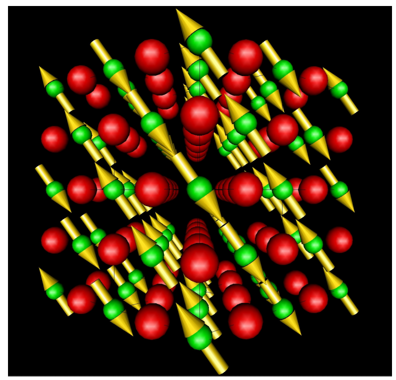
BEC transition temperature is strongly suppressed due to chaining

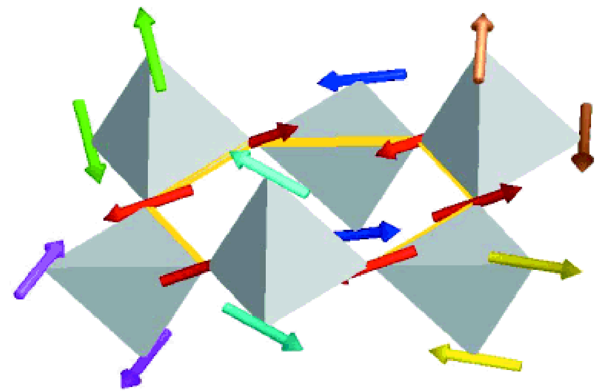
Experimental tests of chaining ???

Quantum magnetism with polar molecules in an optical lattice

Reference: R. Barnett et al., Phys. Rev. Lett. 96:190401 (2006)

Quantum magnetism in solid state systems



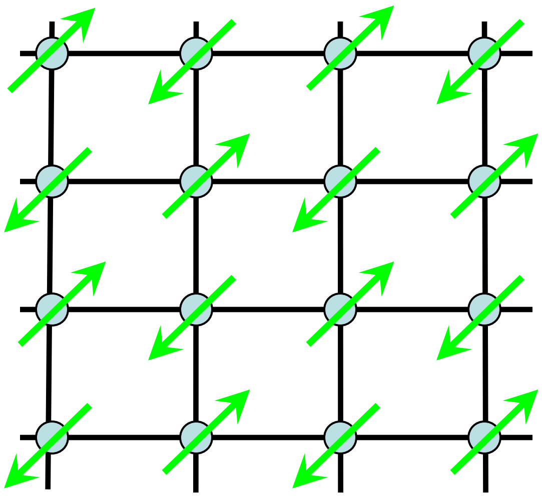


Ferromagnetism in iron

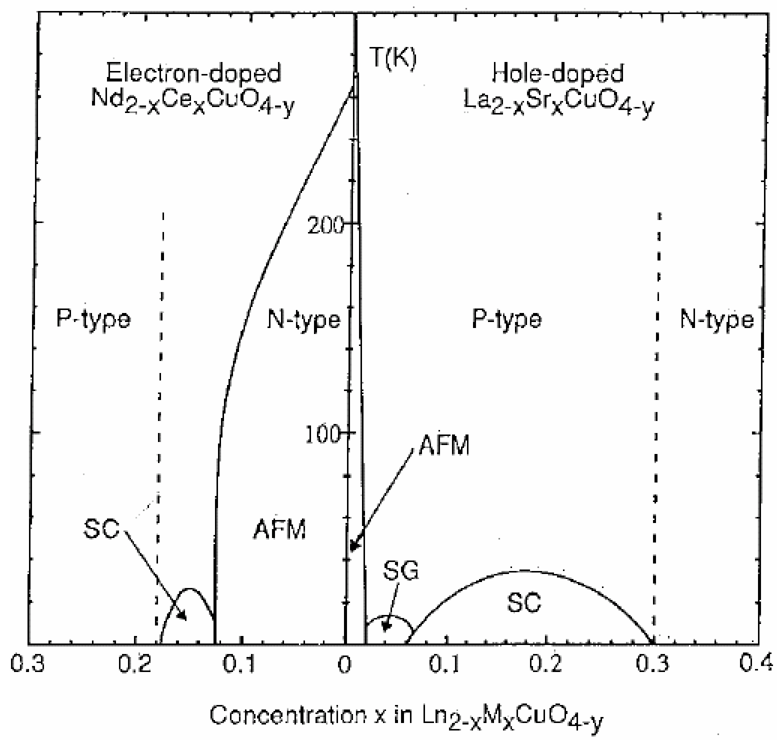
Antiferromagnetism
In MnO2

Frustrated magnetism
in pyrochlore lattice

Antiferromagnetism in high Tc cuprates



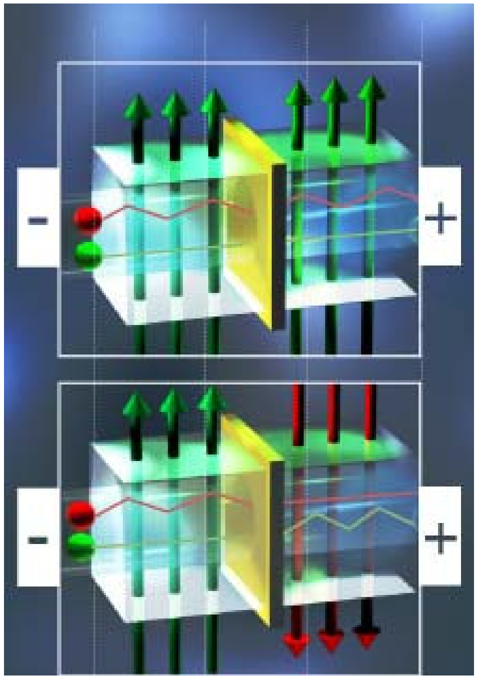
Maple, JMMM 177:18 (1998)



High temperature superconductivity in cuprates is always found near an antiferromagnetic insulating state

Applications of magnetic materials

Magnetic memory in hard drives. Storage density of hundreds of billions bits per square inch.



Magnetic Random Access Memory

Modeling quantum magnetic systems using cold atoms

Controlled collisons of atoms in optical lattices
Jaksch et al. 1999, Mandel et al. 2003

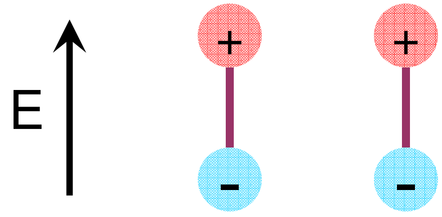
Interacting fermions in special types of lattices
Damski et al. 2005

Exchange interactions of atoms in optical lattices
Duan et al, 2003; Kuklov et al. 2004

Trapped ions interacting with lasers
Deng et al., 2005

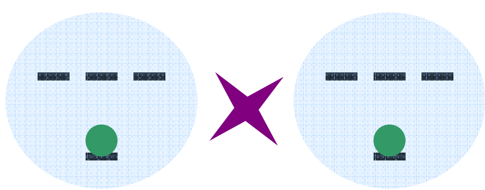
And many more …

Dipolar interactions of polar molecules

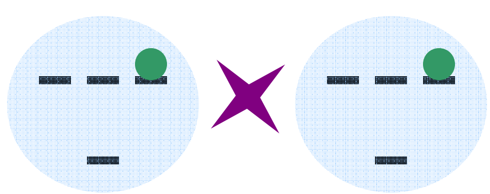


External electric field induces classical dipolar moments in molecules

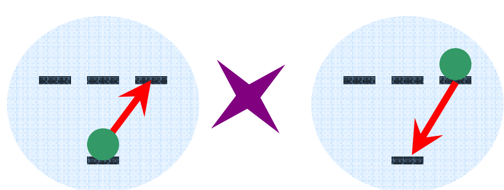
Molecules with well defined angular momentum do not have classical dipolar moments



No dipolar interaction



No dipolar interactionc



Dipolar $1/r^3$ interaction by exchange of angular momentum quanta

Exchange of angular momentum as spin interaction

$$|\,\Psi(t)\,\rangle = \alpha \left|\quad\right\rangle + \beta \cdot e^{-i\Omega t} \left|\quad\right\rangle$$

$$d_x(t) = \alpha^* \beta \cdot e^{-i\Omega t} + \beta^* \alpha \cdot e^{i\Omega t}$$

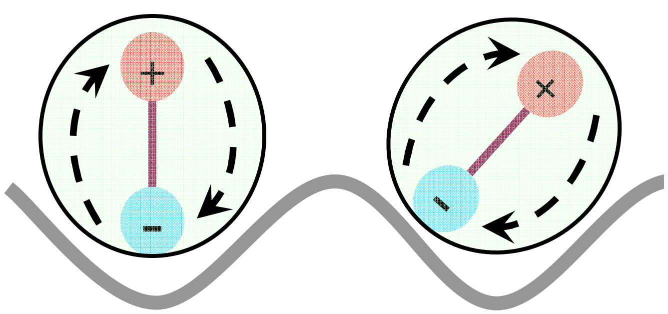
$$d_y(t) = \frac{\alpha^* \beta}{i} \cdot e^{-i\Omega t} - \frac{\beta^* \alpha}{i} \cdot e^{i\Omega t}$$

Precessing dipolar moment

$$|\,\Psi(t)\,\rangle = \alpha \left|\quad\right\rangle + \beta \cdot e^{-i\Omega t} \left|\quad\right\rangle$$

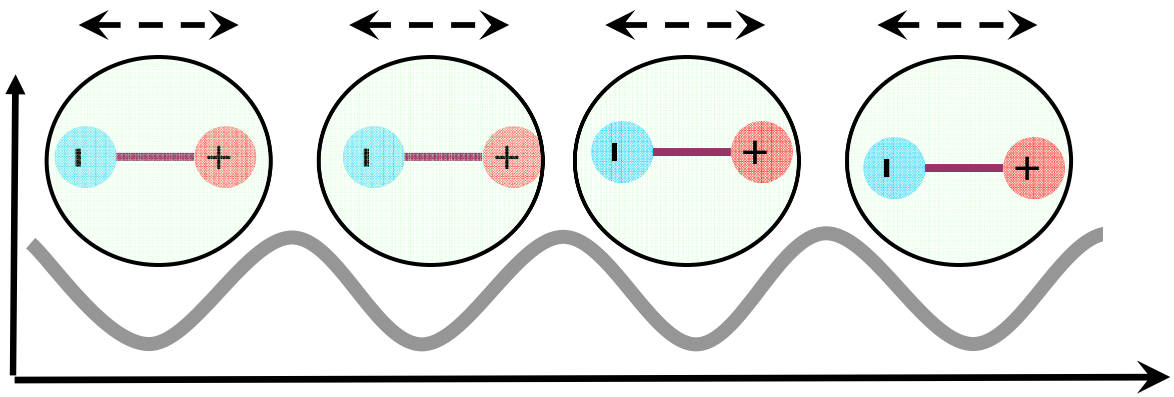
$$d_z(t) = \alpha^* \beta \cdot e^{-i\Omega t} + \beta^* \alpha \cdot e^{i\Omega t}$$

Oscillating dipolar moment

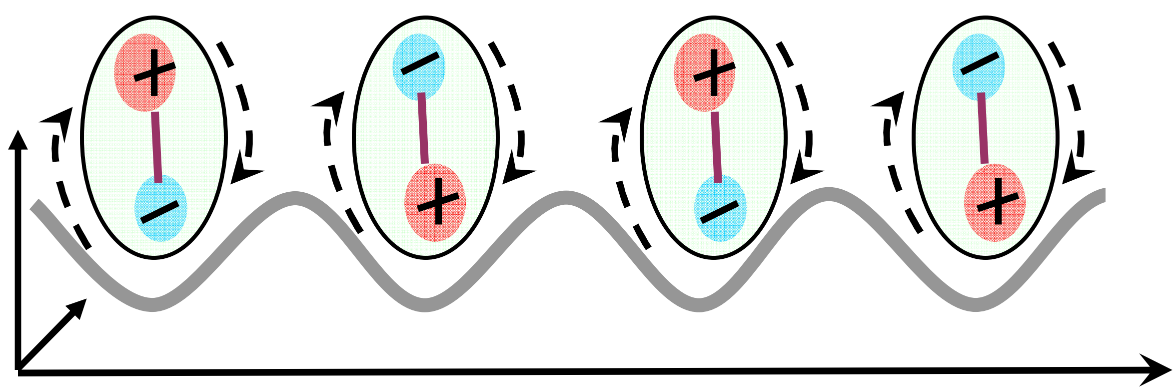


Spin interactions correspond to locking of the relative phase of precession

Spin ordering

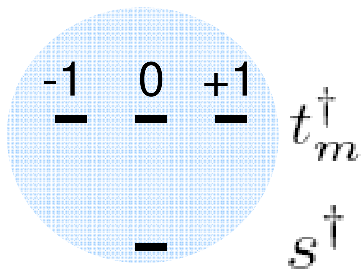


Lattice direction in the plane of dipolar oscillation.
Ferromagnetic ordering



Lattice direction perpendicular to the plane of dipolar precession.
Antiferromagnetic ordering

General approach

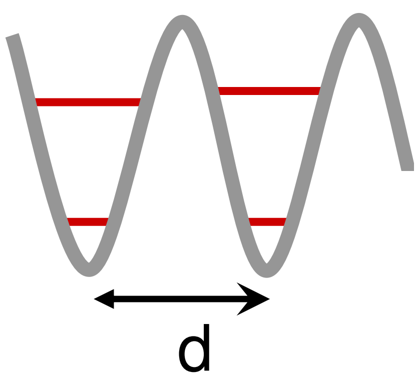


Prepare a mixture of molecules with L=0 and L=1

Alternative basis
(vector representaion)

$$t_x^\dagger = \frac{1}{\sqrt{2}}\left(t_{+1}^\dagger + t_{-1}^\dagger\right) \quad t_y^\dagger = \frac{-i}{\sqrt{2}}\left(t_{+1}^\dagger - t_{-1}^\dagger\right) \quad t_z^\dagger = t_0^\dagger$$

Use one band Hubbard model to describe polar molecules in an optical lattice

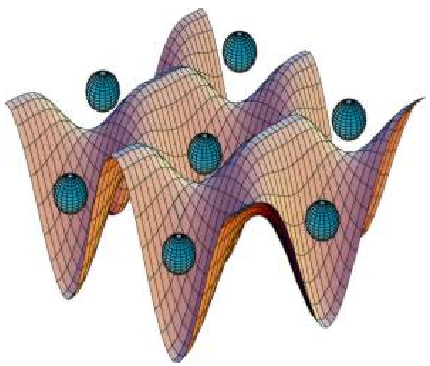


$$\frac{\hbar^2}{md^2} > \frac{D^2}{d^3}$$

$$d > \frac{mD^2}{\hbar^2} = r^*$$

CO r^* = 5.1 nm LiNa r^* = 140 nm KRb r^* = 700 nm

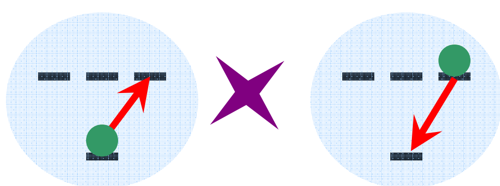
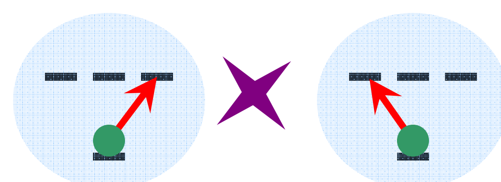
Spin interactions in a Mott phase



$$\mathcal{H}_{\rm dip} = \gamma \sum_{i \neq j} \frac{\vec{d}_i \cdot \vec{d}_j - 3(\vec{d}_i \cdot \vec{e}_{ij})\,(\vec{d}_j \cdot \vec{e}_{ij})}{R_{ij}^3}$$

$$d_{i\alpha} = s_i^\dagger t_{i\alpha}\, e^{-i\Omega t} + t_{i\alpha}^\dagger s_i\, e^{i\Omega t}$$

Neglect terms oscillating at $\pm 2\,\Omega$

Include  but not 

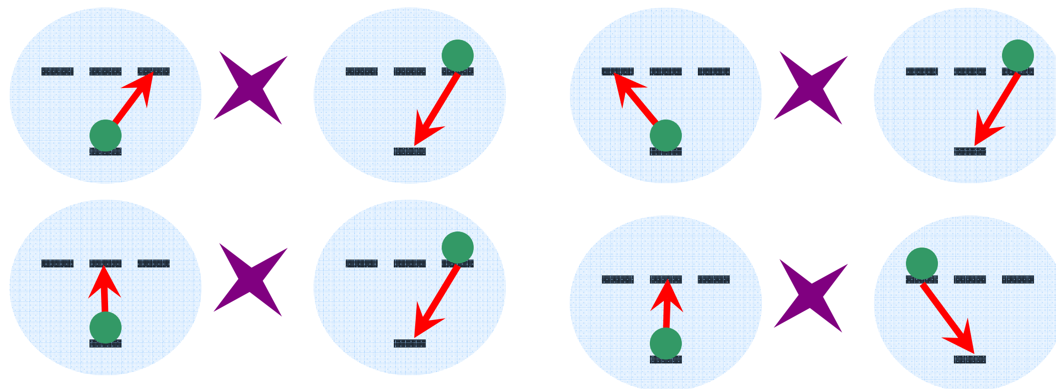
$$\mathcal{H}_{\rm dip} = \gamma \sum_{i \neq j} \frac{(\, s_i^\dagger t_{j\alpha}^\dagger s_j t_{i\beta} + \mathrm{H.c.}\,)\,(\,\delta_{\alpha\beta} - 3 e_{ij\alpha} e_{ij\beta}\,)}{R_{ij}^3}$$

Numbers of L=1 and L=0 molecules are conserved separately

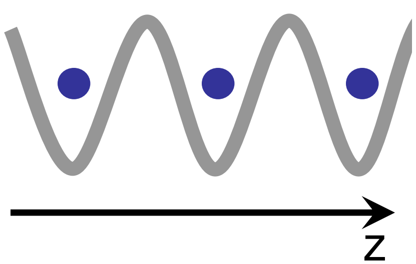
Spin interactions in a Mott phase

$$\mathcal{H}_{\rm dip} = \gamma \sum_{i \neq j} \frac{(\, s_i^\dagger t_{j\alpha}^\dagger s_j t_{i\beta} + \mathrm{H.c.}\,)\,(\, \delta_{\alpha\beta} - 3 e_{ij\alpha} e_{ij\beta}\,)}{R_{ij}^3}$$

Generally, mixing of all (L=1,L_z) is allowed



For certain geometries, there are additional conservation laws. Example:



One dimensional optical lattice in the z direction.
Conserved quantities

$$N_m = \sum_i t_{im}^\dagger t_{im} \qquad N_\alpha = \sum_i t_{i\alpha}^\dagger t_{i\alpha}$$

$$m = \pm 1,\, 0 \qquad \alpha = x,\, y,\, z$$

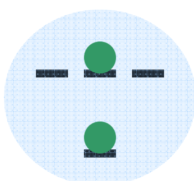
Variational wavefunction

$$|\Psi\rangle = \prod_i \left(\cos\theta \, s_i^\dagger + \sin\theta \sum_\alpha \psi_{i\alpha} t_{i\alpha}^\dagger \right) |0\rangle$$

θ is fixed by the number of L=0 and L=1 molecules

Minimize with respect to $\psi_{i\alpha}$ keeping track of conservation laws

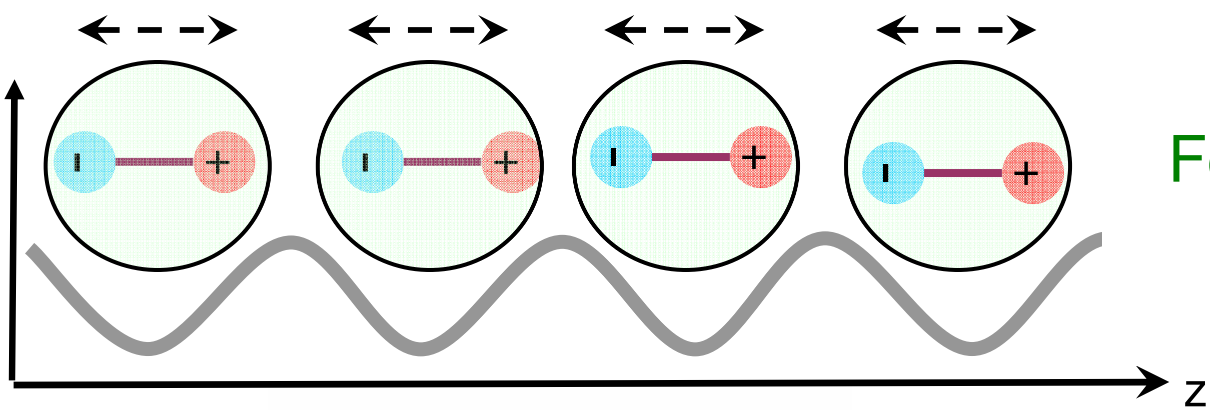
Examples of spin ordering in 1d



$N_z \neq 0$

$N_x = 0$

$N_y = 0$

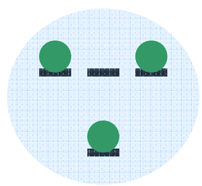


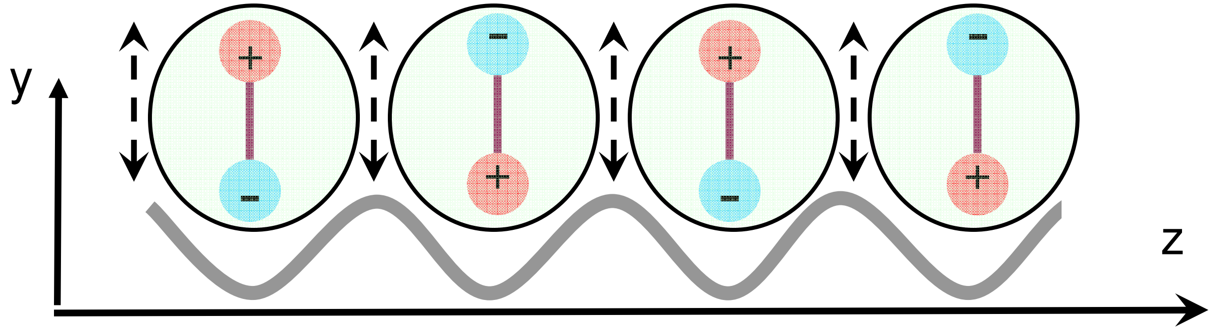
Ferro

$$d_z(i, t) = d_0 \cos \Omega t$$

$$d_x = 0 \qquad d_y = 0$$

Examples of spin ordering in 1d





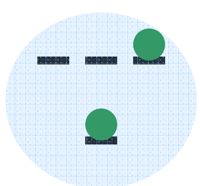
$N_y \neq 0$

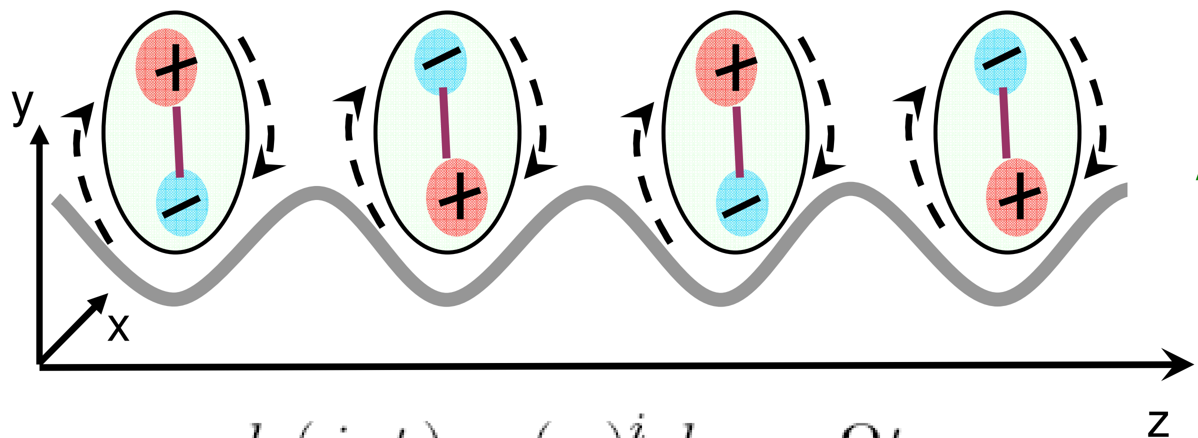
$N_x = 0$

$N_z = 0$

$$d_y(i,t) = (-)^i\, d_0 \cos \Omega t$$

$$d_x = 0 \qquad d_z = 0$$





Antiferro

$N_{+1} \neq 0$

$N_0 = 0$

$N_{-1} = 0$

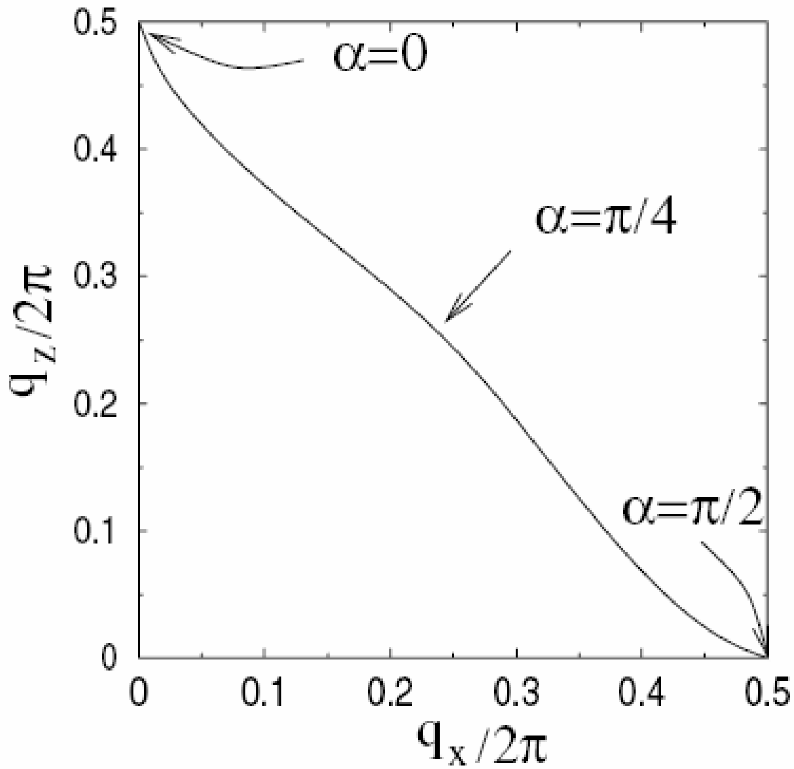
$$d_x(i,t) = (-)^i\, d_0 \cos \Omega t$$

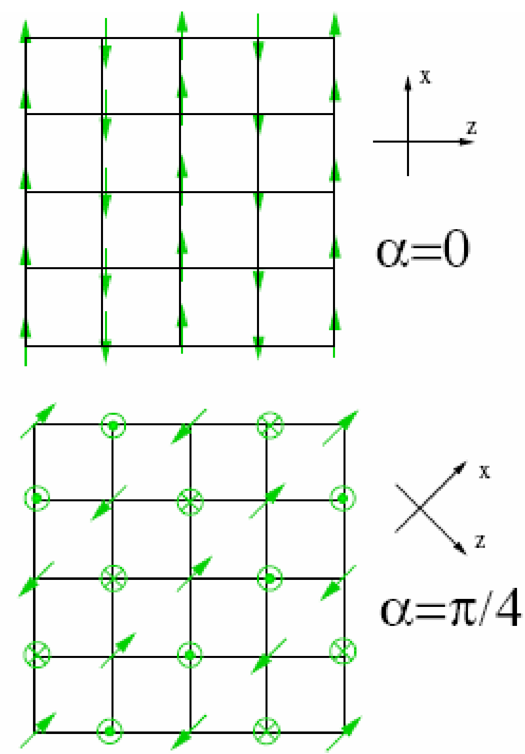
$$d_y(i,t) = (-)^i\, d_0 \sin \Omega t$$

$$d_z = 0$$

Spin ordering in 2d lattices

Molecules prepared as a mixture of L=0 and (L=1,L_Z=+1) states.
Optical lattice in the XZ plane with orientation specified by α





Melting Mott insulators

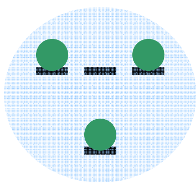
$$\mathcal{H} = \mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{Hub}} + \mathcal{H}_{\text{dip}}$$

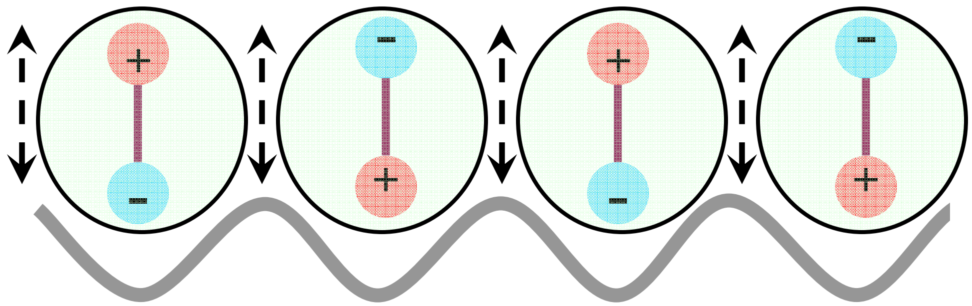
$$\mathcal{H}_{\text{kin}} = -J \sum_{\langle ij \rangle} s_i^\dagger s_j - J \sum_{\langle ij \rangle \alpha} t_{i\alpha}^\dagger t_{j\alpha}$$

$$\begin{aligned}\mathcal{H}_{\text{Hub}} &= U \sum_i n_{si} \left(n_{si} - 1 \right) + \sum_{i\alpha} U_\alpha n_{t_\alpha i} \left(n_{t_\alpha i} - 1 \right) \\ &+ \sum_{i\alpha \neq \beta} U_{\alpha\beta} \, n_{t_\alpha i} \, n_{t_\beta i} + \sum_{i\alpha} V_\alpha \, n_{si} \, n_{t_\alpha i}\end{aligned}$$

$$\mathcal{H}_{\text{dip}} = \gamma \sum_{i \neq j} \frac{\left(s_i^\dagger t_{j\alpha}^\dagger s_j t_{i\beta} + \text{H.c.} \right) \left(\delta_{\alpha\beta} - 3 e_{ij\alpha} e_{ij\beta} \right)}{R_{ij}^3}$$

Melting Mott insulators





$$N_y \neq 0$$
$$N_x = 0$$
$$N_z = 0$$

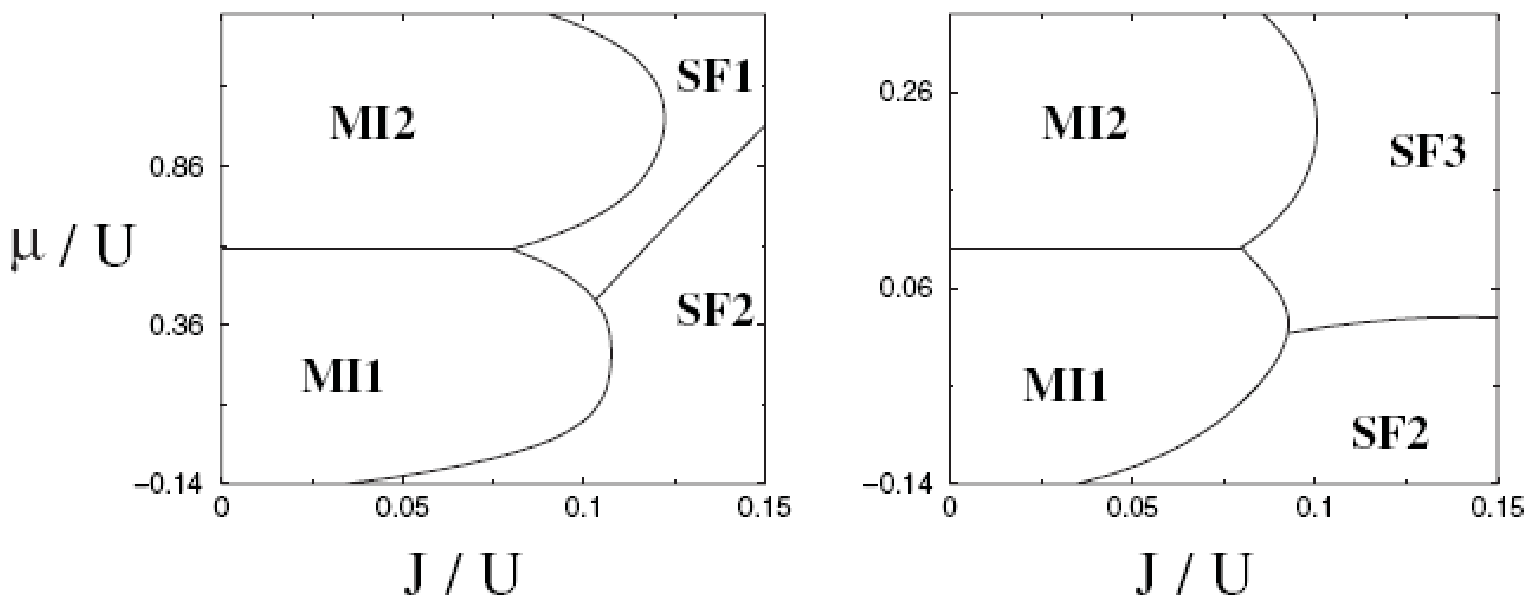
$$d_y(i, t) = (-)^i \, d_0 \cos \Omega t$$

$$d_x = 0 \qquad d_z = 0$$

Competition between kinetic energy and dipolar interactions.
Kinetic energy favors condensation all particles at q=0.
Dipolar interaction energy is minimized when the relative mometum between *s* and *t* molecules is π.

Melting Mott insulators

Two dimensional systems. Phase diagrams for various values of Hubbard interactions. All Mott phases have spin orer at (π, π)



SF1 partial phase separation. Dipolar ordering stays at π

SF2 complete phase separation into *s* and *t* molecules

SF3 ordering wavevector continuously changes from (π, π) to 0

Spin interactions in systems of polar molecules

Have large energy scale

Long ranged

Anisotropic

Can be used for understanding (anti)ferroelectric systems.
This is important for modern technologies (e.g. FRAM)

Can be used for modeling systems with exotic spin order
(beyond mean-field factorizable wavefunctions)

Quantum melting of spin ordered Mott phases of polar molecules
gives rise to very interesting superfluid phases