cond-mat/0607294

# 2D Self-Assembled Crystals with Polar Molecules: Shaping the Interaction Potentials

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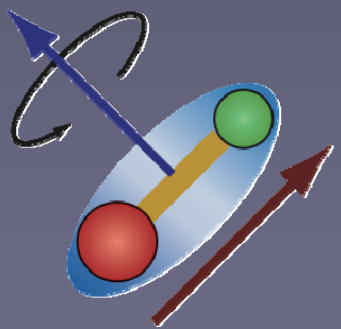


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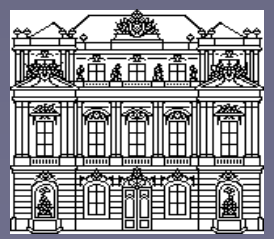

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# Quantum degenerate gases of bosons and fermions

***dilute*** atomic/molecular gases

**Bose-Einstein condensation**

- Gross-Pitaevskii equation
- non-linear dynamics

**Rotating condensates**

- vortices
- fractional quantum Hall

**Molecules**

- Feshbach resonances
- BCS-BEC crossover
- polar molecules

**Optical lattices**

- quantum information
- Hubbard models
- strong correlations
- exotic phases

**control and tunability**

new tools

novel interesting many-body physics

# Polar Molecules

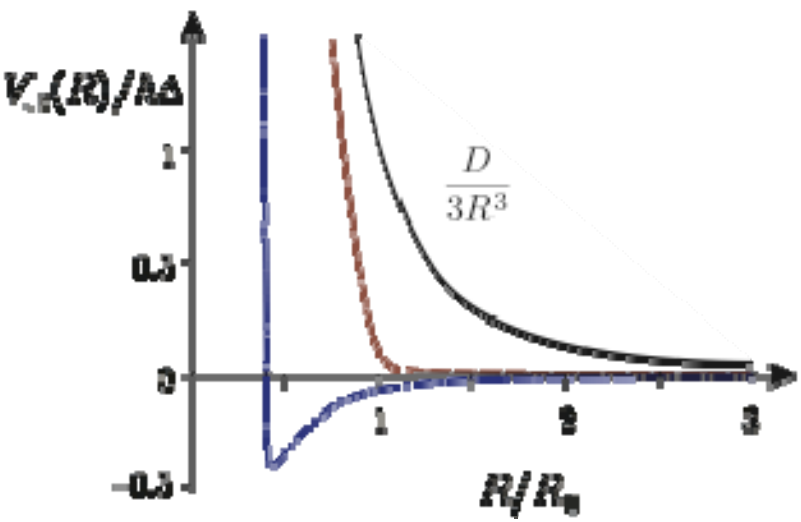
## Why polar molecules?

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

## Polar molecules in 2D

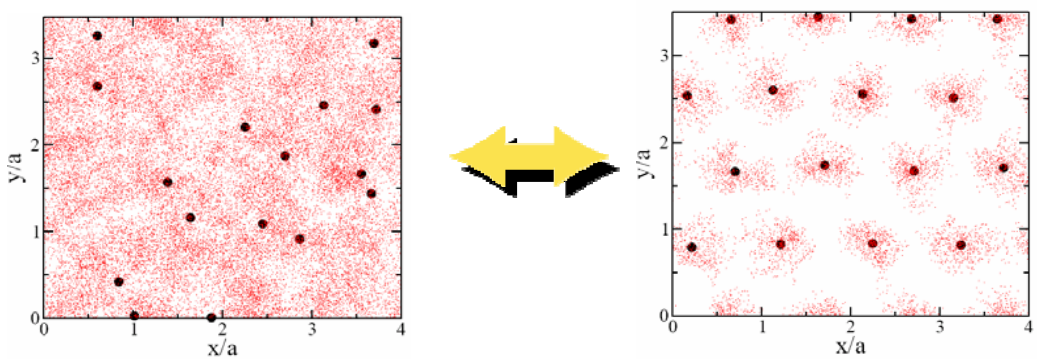
- stability for strong interactions
  - suppressed three-body recombination
- tunable long range interaction in ***strength*** and ***shape***
- tool for exploring novel quantum phenomena

## Tunable interaction




## Self-Assembled Crystals

- superfluid/crystal quantum phase transition



# Polar Molecules

## Why polar molecules?

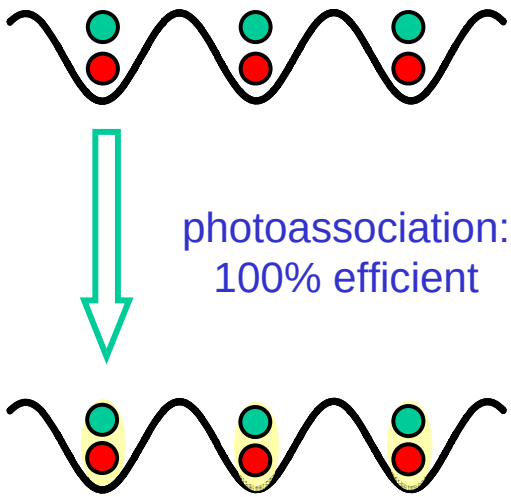
- coupling to optical and microwave fields
  - cooling/trapping
  - internal states
- permanent dipole moment
  - strong dipole-dipole interaction
  - long-range interaction

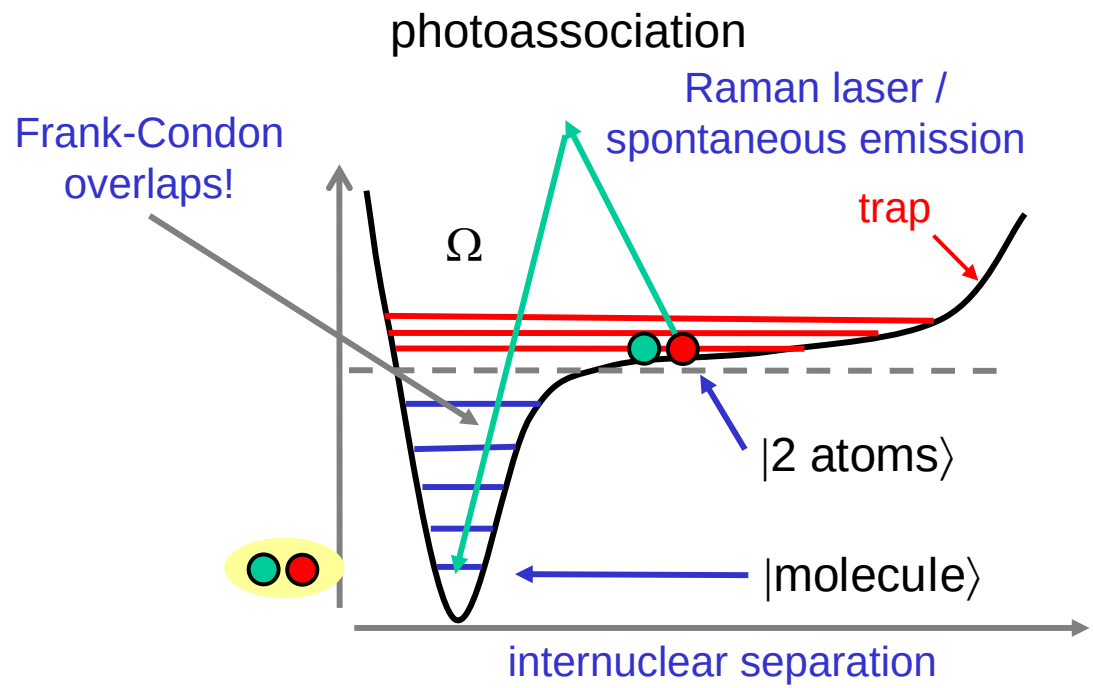
## What polar molecules?

-$X^1\Sigma$ closed shell (SrO, CsRb)

- *Electronic and vibrational ground state*

- Preparation by:
  - Buffer-gas cooling
  - Photoassociation (e.g. from two-species BEC )



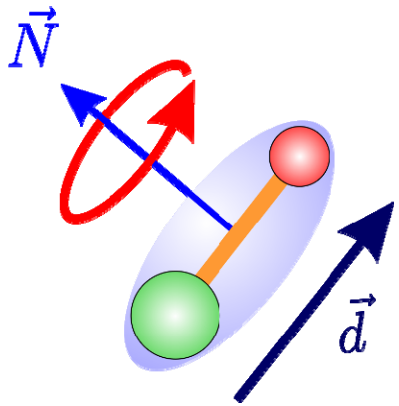



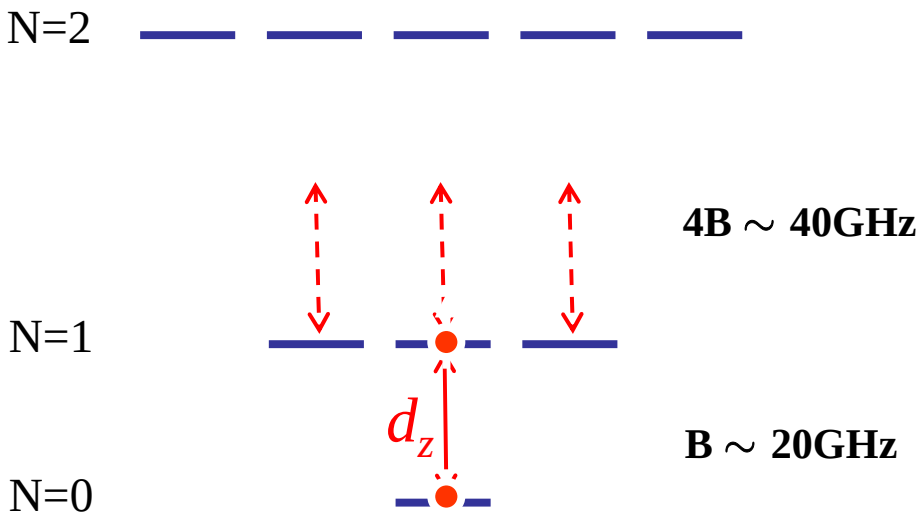
# Design of inter-particle interactions

# Single polar molecule: Rotational spectroscopy

Rigid Rotor:

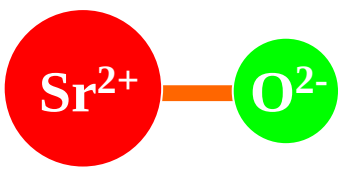
$$H = B\,\mathbf{N}^2$$




"charge qubit"

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




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

# Interaction between two polar molecules

Hamiltonian

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

kinetic energy | trapping potential | rigid rotor | electric field | interaction potential

Dipole-dipole potential

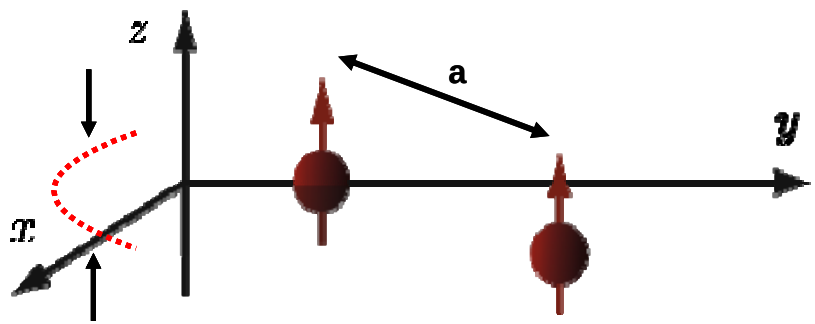
- E=0: van der Waals attraction in the ground state

$$C_6 \approx d^4/6B$$

$$V_{\text{vdW}} \sim -C_6/r^6$$

Trapping potential

- strong transverse trapping confining the system into 2D




Tune the interaction between polar molecules

(i) static electric field

(ii) microwave fields

# Static Electric Field

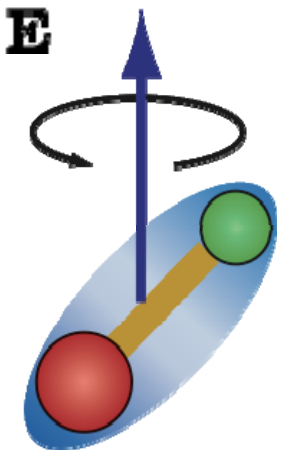
## Dipole moment (single molecule)

-electric field along the z-axis “alignes” the molecules

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

- finite averaged dipole moment in |g>

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

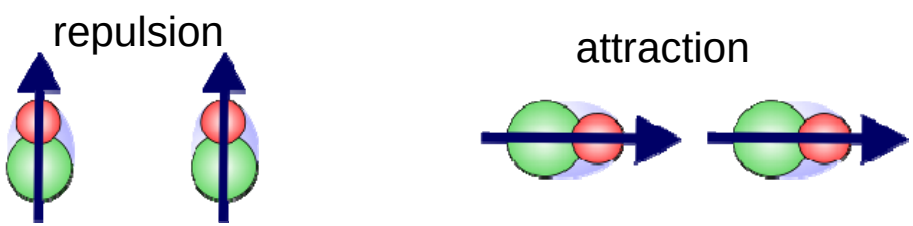



## Dipole-dipole interaction

-long-range interaction

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

-anisotropic interaction




attraction — Instability in the many-body system

# Static Electric Field: Collisional Stability

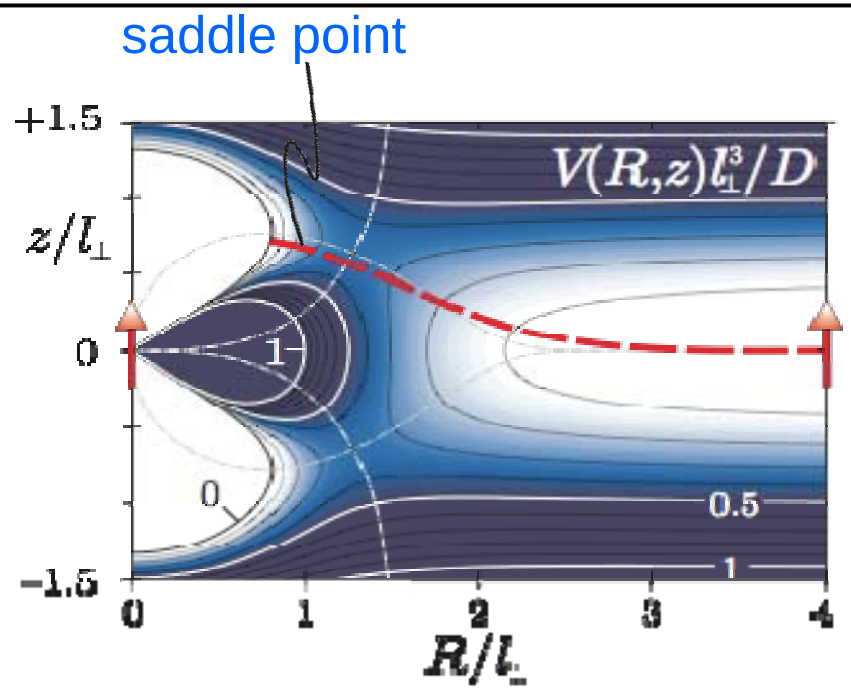
## Effective interaction

- interaction potential with transverse trapping potential

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

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

- potential barrier: larger than kinetic energy → collisional stability



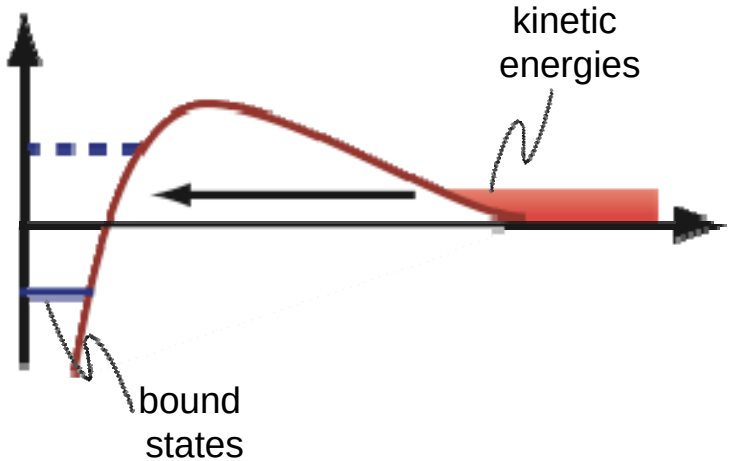

## Tunneling rate:

attempt frequency

- semi-classical rate (instanton techniques) $\Gamma = A\exp\left(-S_E/\hbar\right)$

- Euclidean action of the instanton trajectory $S_E = \hbar\left(\frac{Dm}{\hbar^2 a_\perp}\right)^{2/5} C$

numerical factor: $C \approx 5.8$



# Effective 2D Interaction Hamiltonian

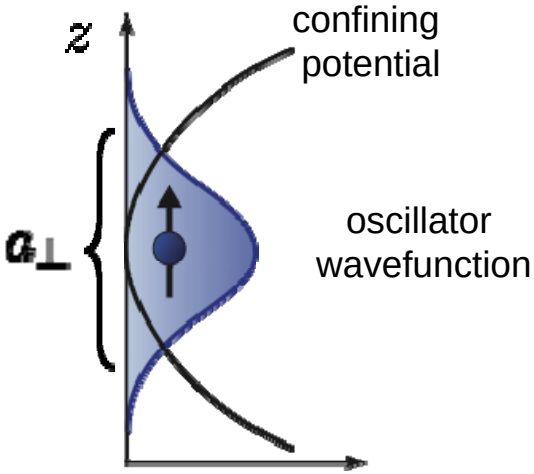
Transverse trapping

- integrating out the fast transverse motion of the molecules

transverse wave function

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

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




Effective 2D potential

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

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

# Microwave field

## Internal dynamics

weak static field

microwave field

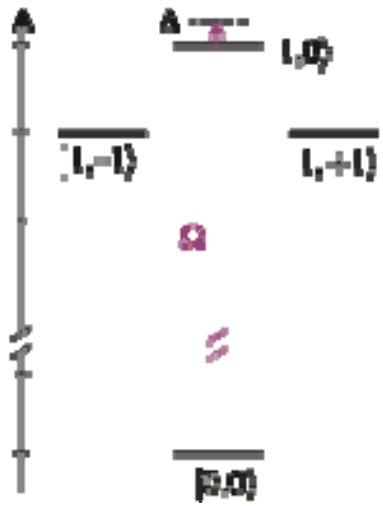
- rigid rotor

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

- Microwave field:

$\Delta$ : detuning

$\Omega$ : Rabi frequency



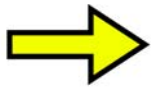
## Interaction

- dipole-dipole interaction between two polar molecuels

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

# Microwave field

Born-Oppenheimer:
- solve the internal dynamics for fixed particle positions
- reduction to two internal states per particle

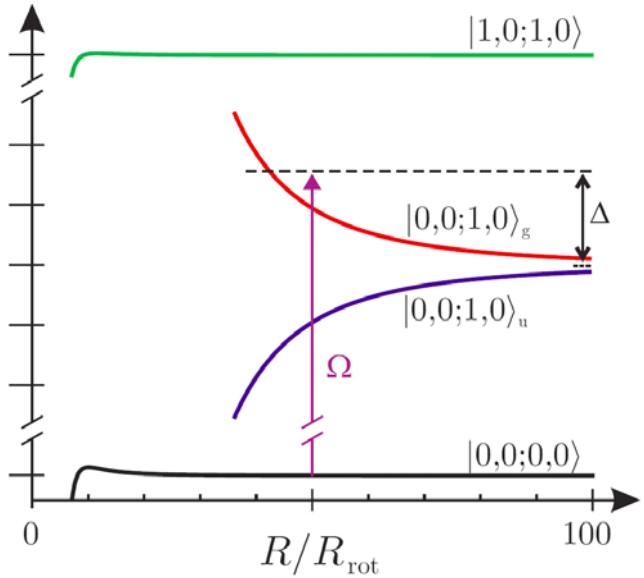


4 state manifold dressed
by the external field

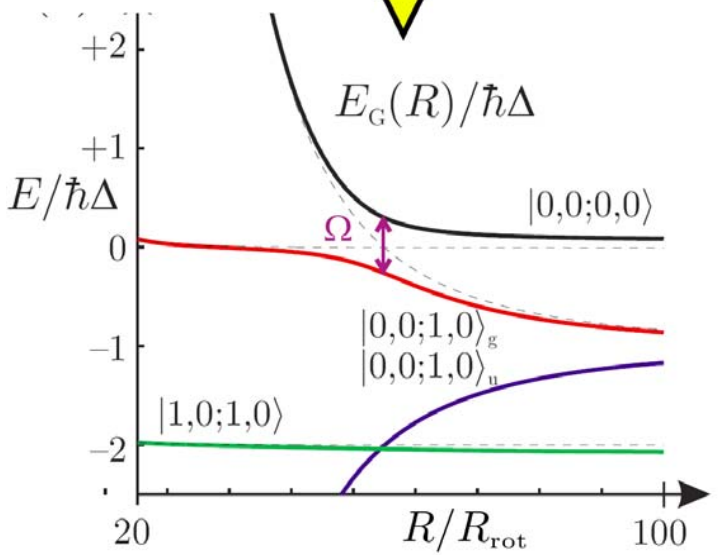
-Rotating frame:

$$H = \begin{pmatrix} 0 & \Omega & \Omega & 0 \\ \Omega & \Delta & d^2/3R^3 & \Omega \\ \Omega & d^2/3R^3 & \Delta & \Omega \\ 0 & \Omega & \Omega & 2\Delta \end{pmatrix}$$

- level crossing at $\Delta = \frac{d^2}{3R_0^3}$



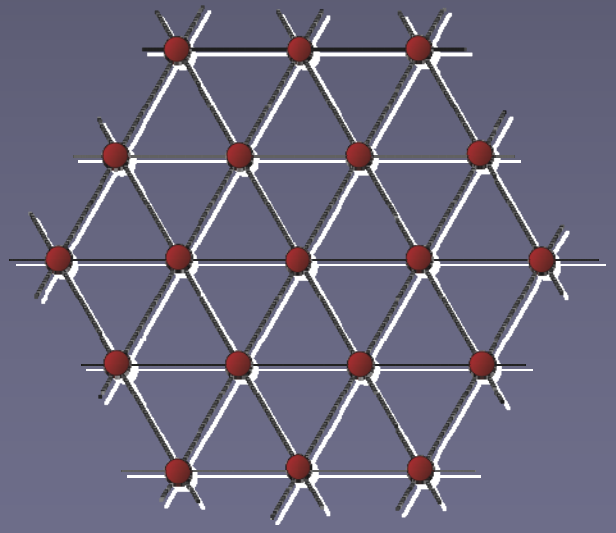

rotating
frame




Effective 2D potential: “Hard Sphere”

$$V_{eff}(R) = \begin{cases} \frac{d^2}{3R^3} & R < R_0 \\ \frac{\Omega^2}{\Delta^2}\frac{d^2}{3R^3} & R > R_0 \end{cases}$$

# Many-Body Physics: The Crystalline phase



# Effective 2D Hamiltonian

## Hamiltonian

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

interaction strength:

$$r_s = \frac{E_{int}}{E_{kin}} = \frac{Dm}{\hbar^2 a}$$

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

## Polar molecule: SrO

- dipole moment:

$$d \sim 9D \quad (2.4\ \text{Debye} \sim e a_0)$$

$$r_s \sim 121 \mu m / a$$

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

- interparticle distance: $a \sim 300 - 500\text{nm}$

- stability: $S_w/\hbar \gtrsim 130$

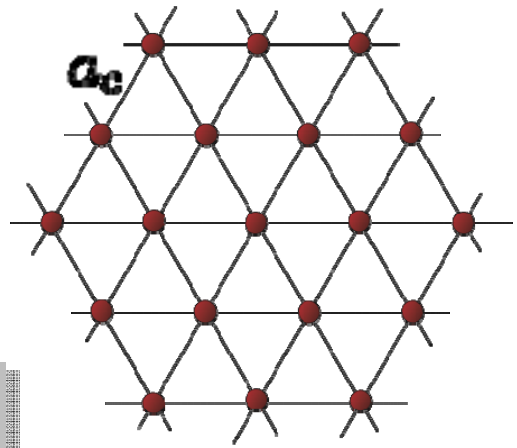
# Crystalline phase

## Strong interactions

- leading order: only keep the interaction term

- describes purely classical problem

- minimization of energy: hexagonal lattice




number of particles

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

numerical prefactor

## Lattice vibrations

- harmonic oscillations around equilibrium: phonon modes

- energy correction due to zero point fluctuations of the phonons

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

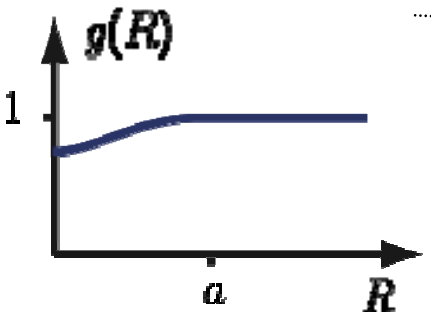
# (Tentative) Phase Diagram

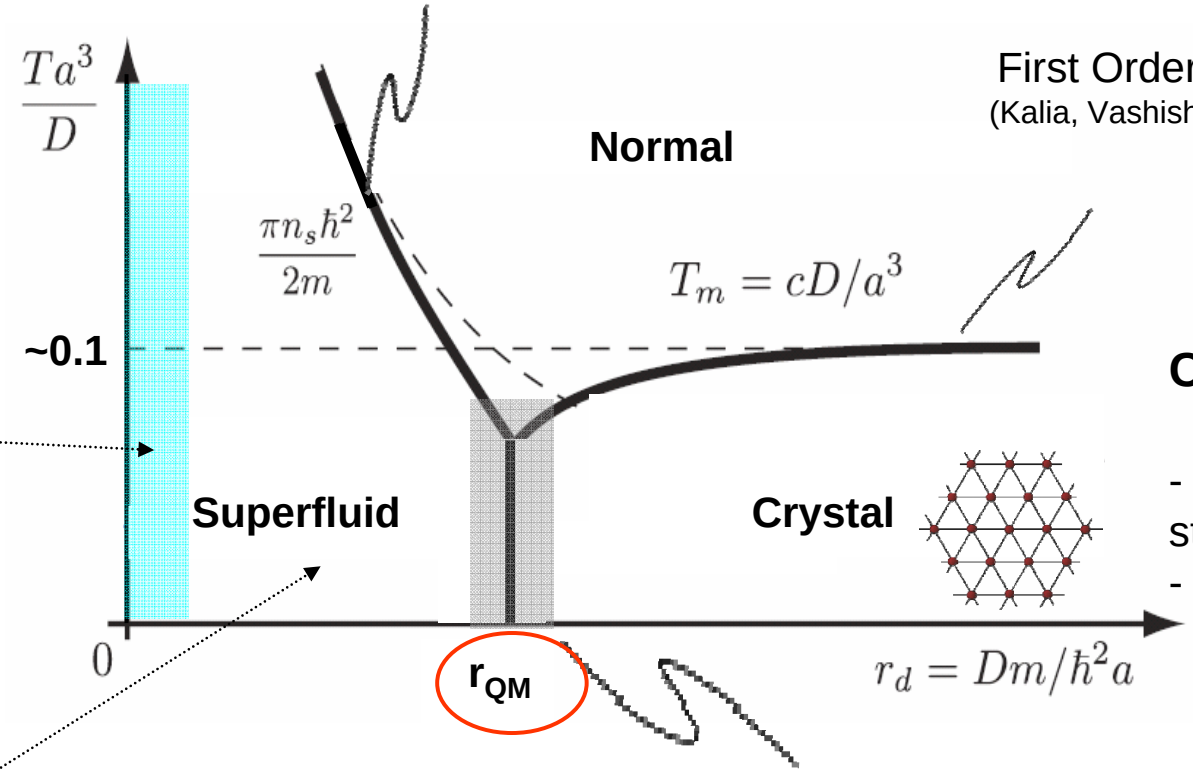
Kosterlitz-Thouless Transition

First Order Transition
(Kalia, Vashishta J.Phys.C 81)

**Weakly interacting superfluid**

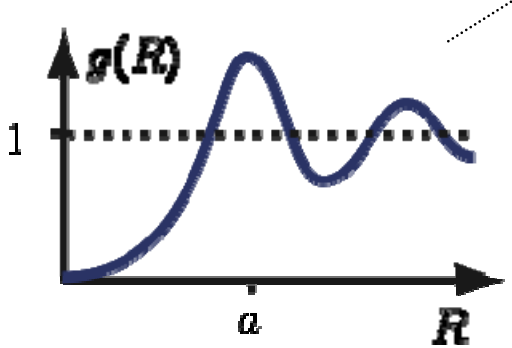
- small quantum depletion
- Bogoliubov theory




**Crystal phase**

- triangular lattice structure
- phonon modes




**Strongly interacting superfluid**

- superfluid stiffness
- large depletion

**Note: many body wave function does not "see"small distances**

Quantum melting

- first order transition? superfluid-crystal
- intermediate phases?
  - supersolids

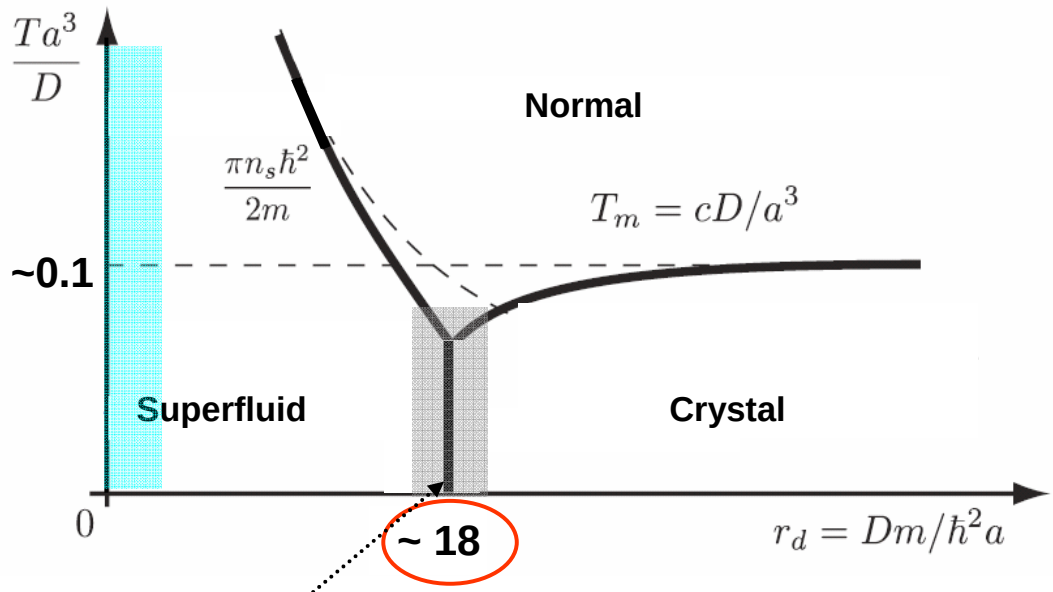
**(PIMC results)**

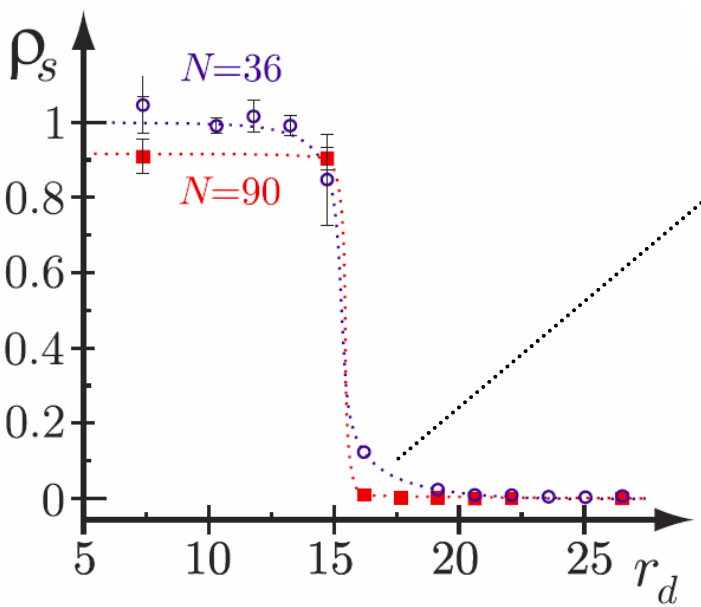
# Quantum Melting

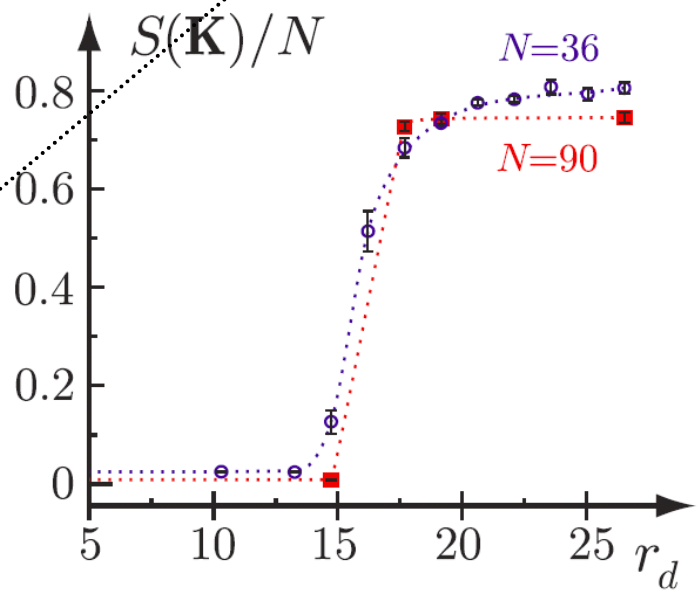
Quantum melting

- first order transition?
  superfluid-crystal
- intermediate phases?
  - supersolids

First order phase transition




PIMC, Worm-Algorith-based code, Boninsegni,Prokof'ev,Svistunov,PRL06

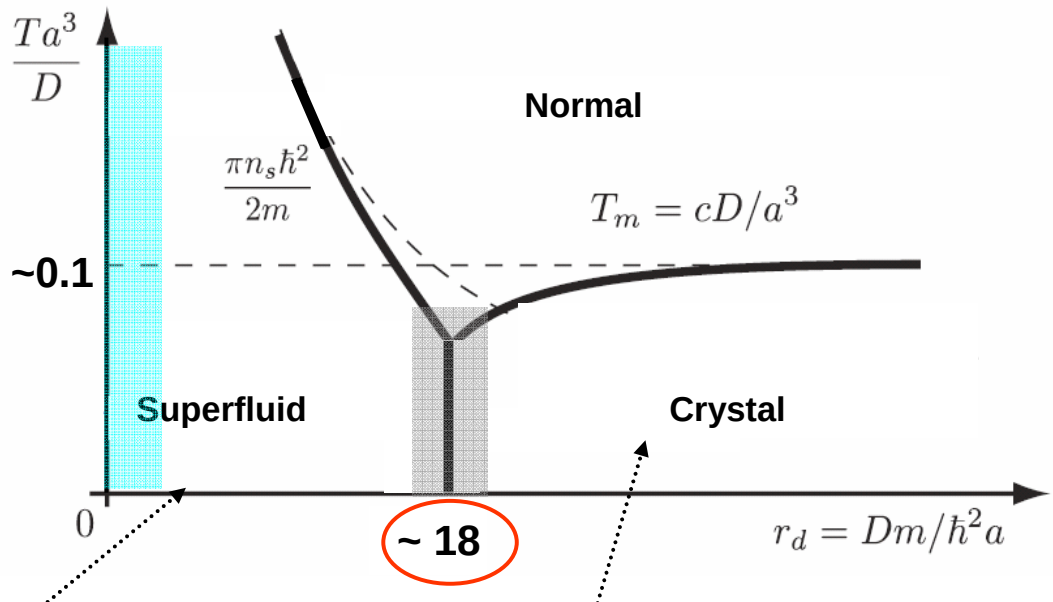
# Quantum Melting

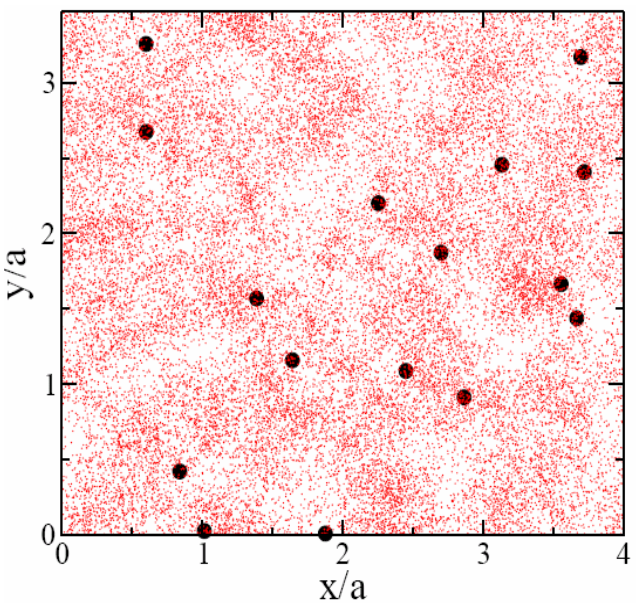
Quantum melting

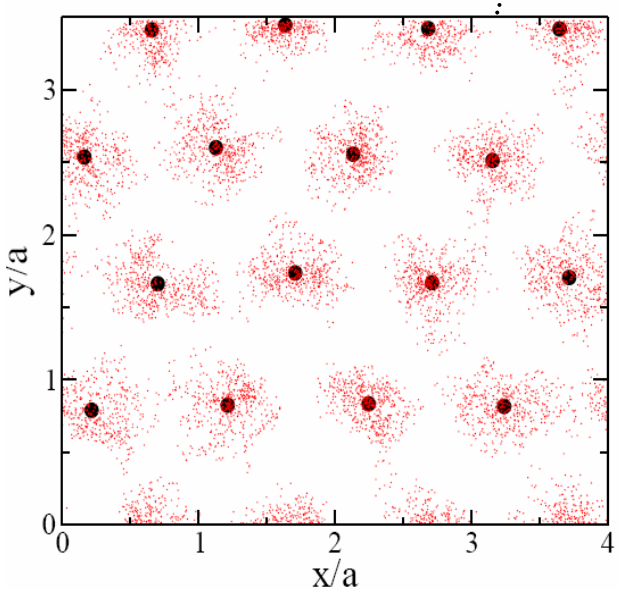
- first order transition?
  superfluid-crystal

- intermediate phases?
  - supersolids

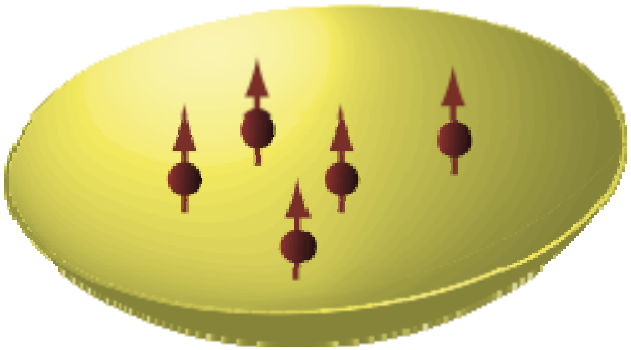
First order phase transition



# Molecules in a trap



$$V_T(\mathbf{R}) = \frac{1}{2} m \omega_T^2 R^2$$

New features

- shell structure

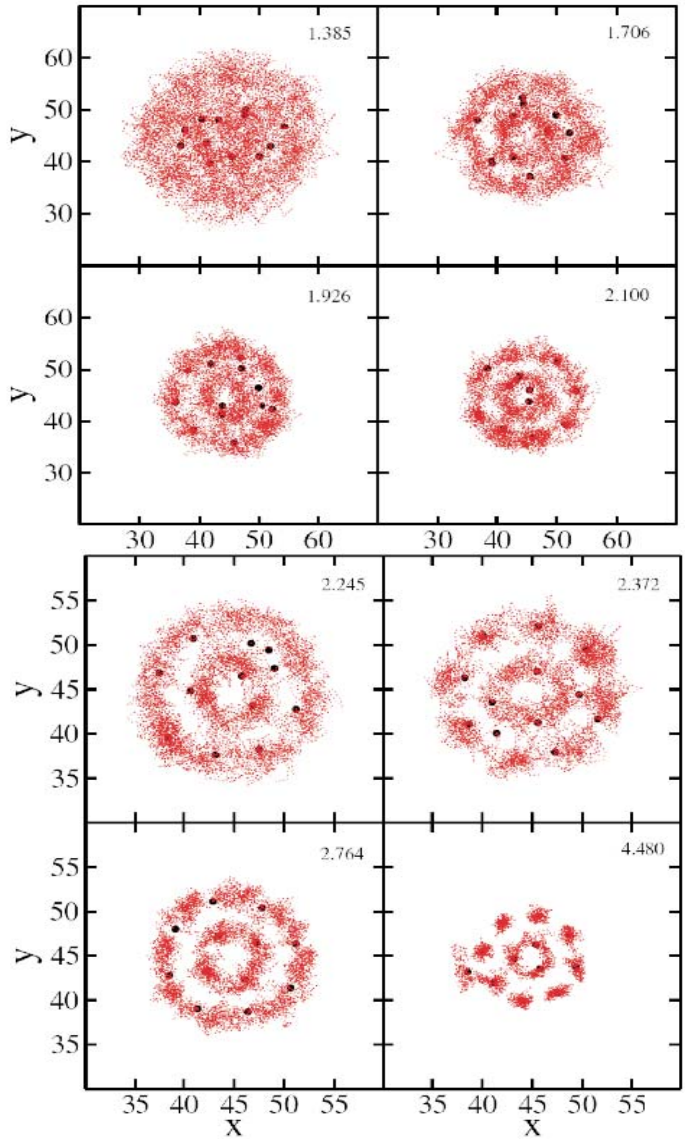
- magic numbers

- two-step melting

- possible different lattice geometries

increasing interaction

appearance of crystaline order

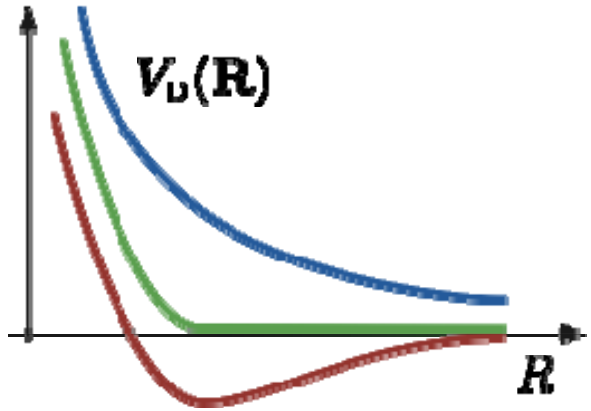


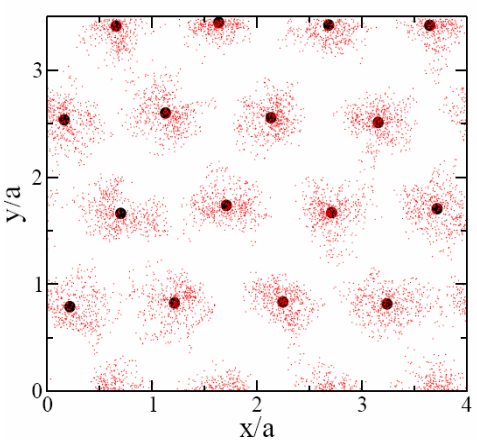
# Conclusions

cond-mat/0607294

## Tunable long-range interaction

- strenght of dipole-dipole interaction
- changing the shape of the
  the potential
- hard-sphere potential



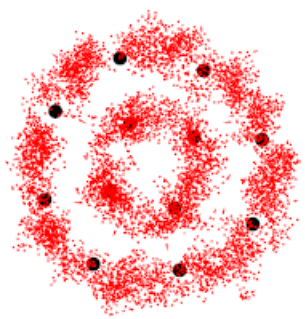



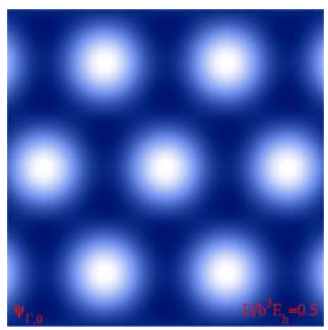

## Polar molecular crystal

- novel phase in cold gases
- linear phonon modes
- tunable lattice parameters
- quantum melting transition

## Outlook

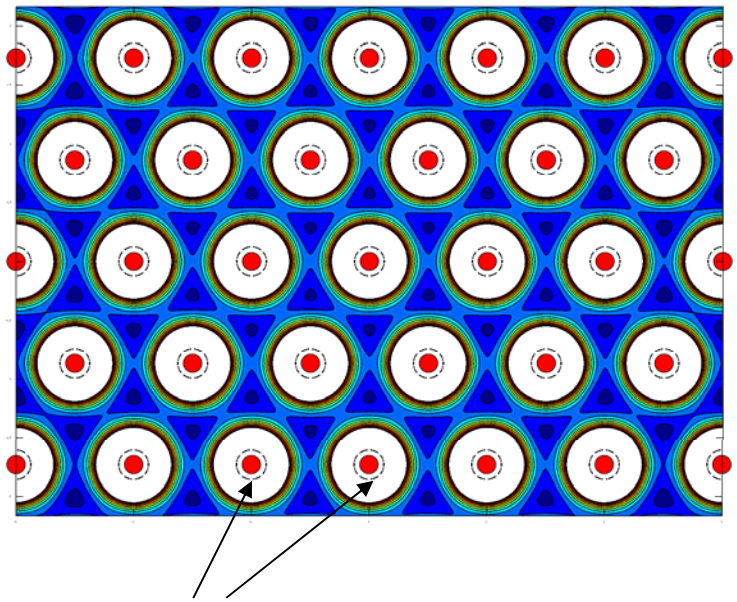
- mesoscopic physics with trapped molecules
- spin lattice toolbox
- lattice for condensed matter simulations
- bi-multi layer





# Potential future applications … ⟺ optical lattices

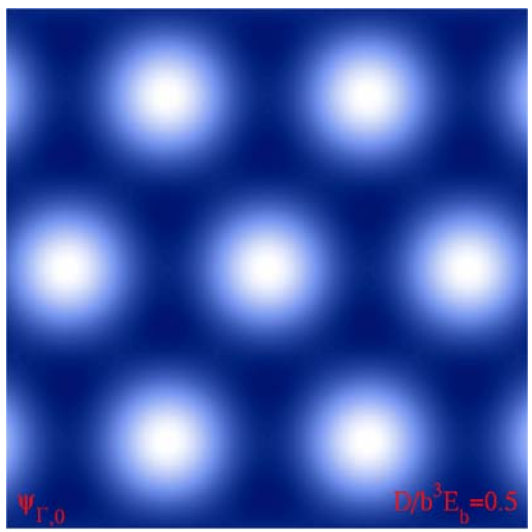
- spin lattice toolbox
  - add spin degree of freedom & engineer spin dependent interactions
- Hubbard models with the new lattices



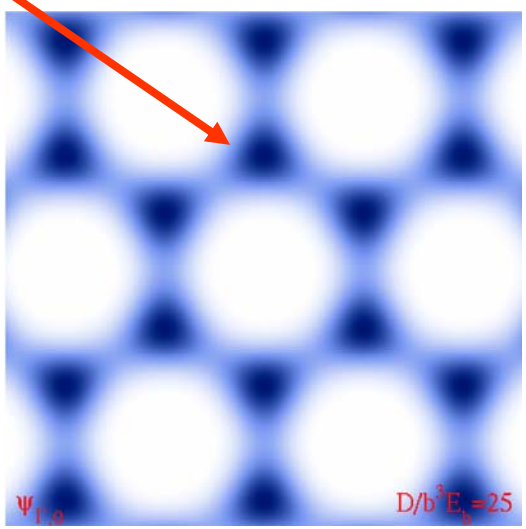
small lattice constants ☺

1. dipoles generate
a 2D periodic lattice
= trap

2. particles moving in this lattice
will see a honeycomb lattice=
Hubbard model




shallow trap: quasi-free



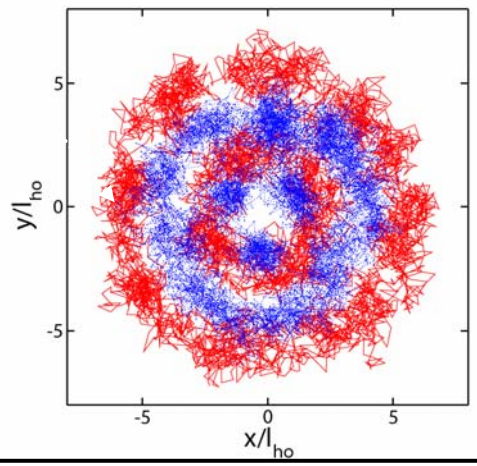

strong trap: tight binding

- bi- and multilayer systems

# Dipolar crystals vs. Optical Lattices

## crystalline phase

tunable lattice spacing
strongly interacting phase
self assembled
phonon modes




## optical lattice

min. lattice spacing fixed
(optical wave-length)
weakly interacting gas
increase of interaction via
quenching of hopping

# Dipolar crystals vs. Wigner crystals

## dipole/1D-2D: ~$d^2/R^3$

$r_d = E_{pot}/E_{kin} = (d^2/R^3)/(\hbar^2/ m R^2) \sim 1 / R$

crystals @ *high* densities
tunable “charge”

## coulomb/3D: ~$e^2/R$

$r_c = (e^2/r) / (\hbar^2/ m R^2) \sim R$

crystals @ low densities