Three-body Interactions in Cold Polar Molecules

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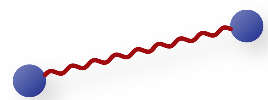
Three-body interactions

Many-body interaction potential

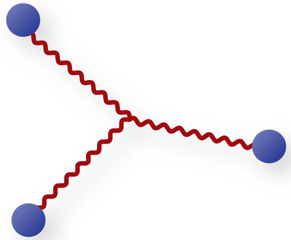
- Hamiltonians in condensed matter are effective Hamiltonains after integrating out high energy excitations

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

two-particle interaction



three-body interaction



Application

- Pfaffian wave function of fractional quantum Hall state (More and Read, ‘91)

- exchange interactions in spin systems: microscopic models exotic phases (Moessner and Sondi, ’01, Balents *et al*., ’02, Moutrich and Senthil ‘02)

- string nets: degenerate Hilbertspace for loop gases (Fidowski, *et al,* ‘06)

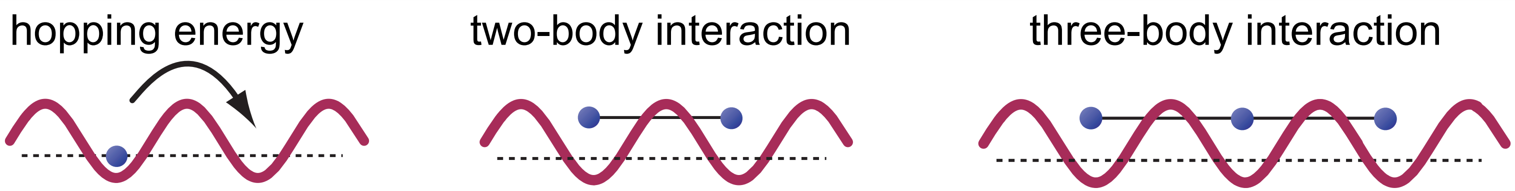
Route towards exotic and topological phases?

Three-body interactions

Extended Bose-Hubbard models

- hardcore bosons

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

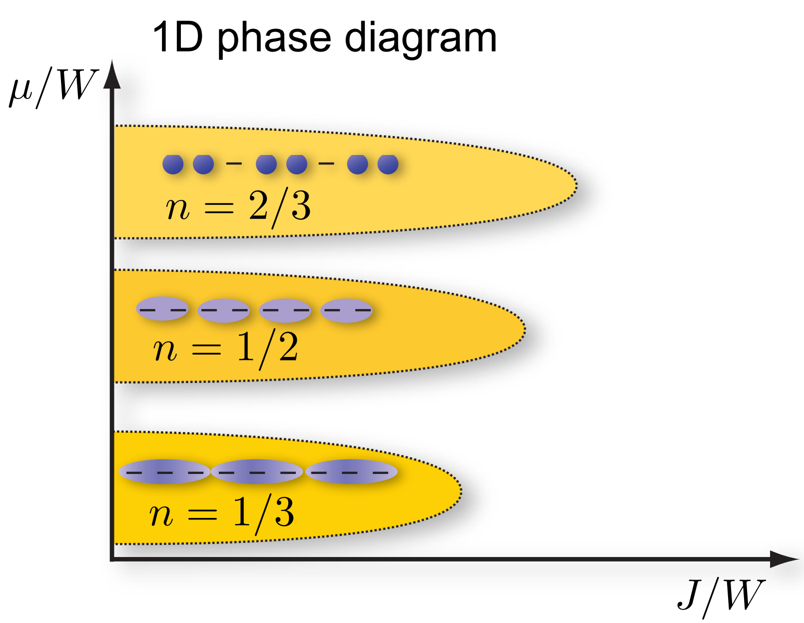


Goal

- large interaction strengths

- independent control of two- and three-body interaction

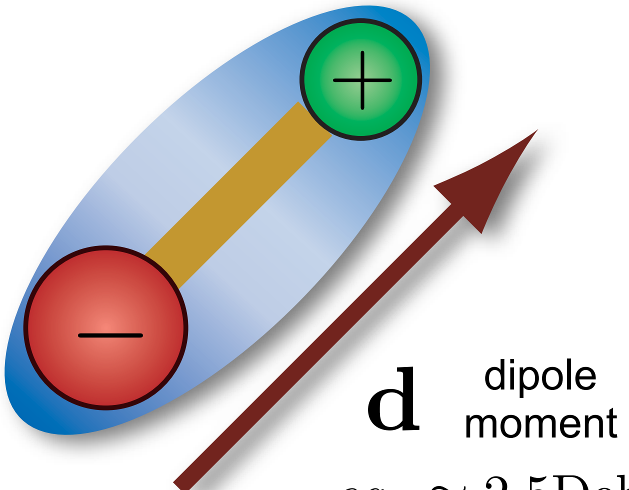
Realizable with polar molecules



Polar molecules

Hetronuclear Molecules

- electronic excitations
  $\sim 10^{15}\mathrm{Hz}$
- vibrational excitations
  $\sim 10^{13}\mathrm{Hz}$
- rotational excitations
  $\sim 10^{10}\mathrm{Hz}$
- electron spin
- nuclear spin



$ea_0 \approx 2.5\mathrm{Debye}$

Polar molecules in the electronic, vibrational, and rotational ground state

- permanent dipole moment: $d \sim 1-9$ Debye
- polarizable with static electric field, and microwave fields

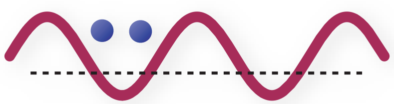
Strong dipole-dipole interactions tunable with external fields

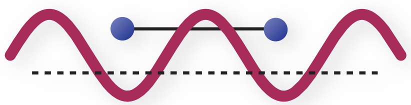
$$V(\mathbf{r}) = \frac{\mathbf{d}_1\mathbf{d}_2}{r^3} - 3\frac{(\mathbf{d}_1\mathbf{r})(\mathbf{d}_2\mathbf{r})}{r^5}$$

Interaction energies

Particles in an optical lattice

- lattice spacing $a = \lambda/2 \sim 500\mathrm{nm}$
- recoil energy $E_r = \dfrac{2\hbar^2\pi^2}{m\lambda^2}$
- size of Wannier function $a_{\mathrm{h.o}} \sim 0.2a$





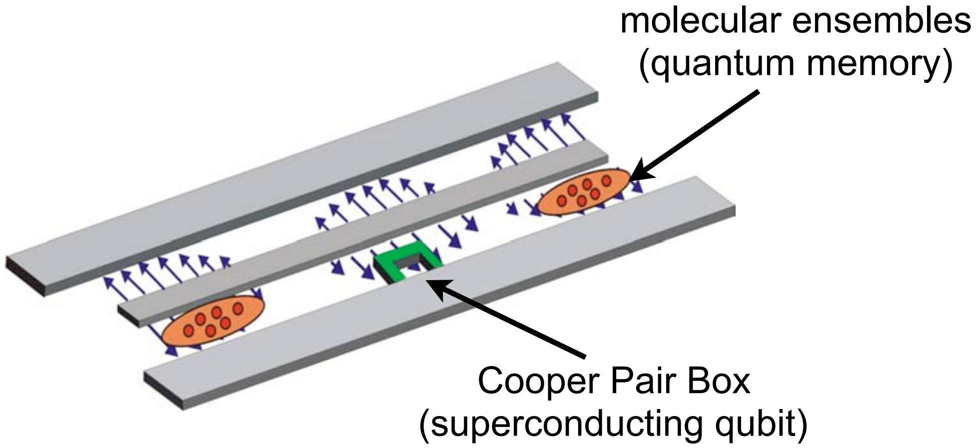
	on-site interaction	nearest-neighbor interaction
Pseudo-potential - dominant interaction in atomic gases	$U \sim 0.5E_r$	present but small
Magnetic dipole moment - Chromium atoms with $m \sim 6\mu_B$	$U \sim 0.5E_r$	$U_1 \sim 10^{-3}E_r$
Electric dipole moment - LiCs hetronuclear molecule $d \sim 6.5\mathrm{Debye}$	$U \sim ???$ $(a/a_{\mathrm{h.o}})^3 U_1$	$U_1 \sim 30E_r$

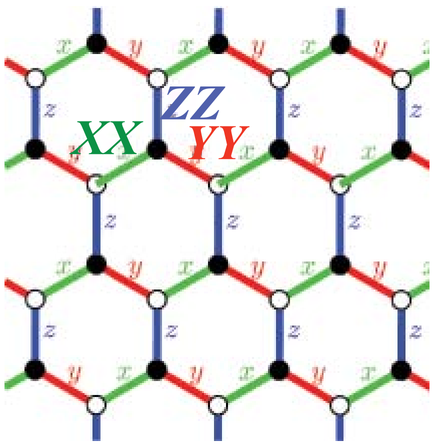
- increased by factor $1/\alpha^2 \sim (137)^2$

Polar molecules

AMO- solid state interface

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





Spin toolbox

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

Polar molecules

Experimental status

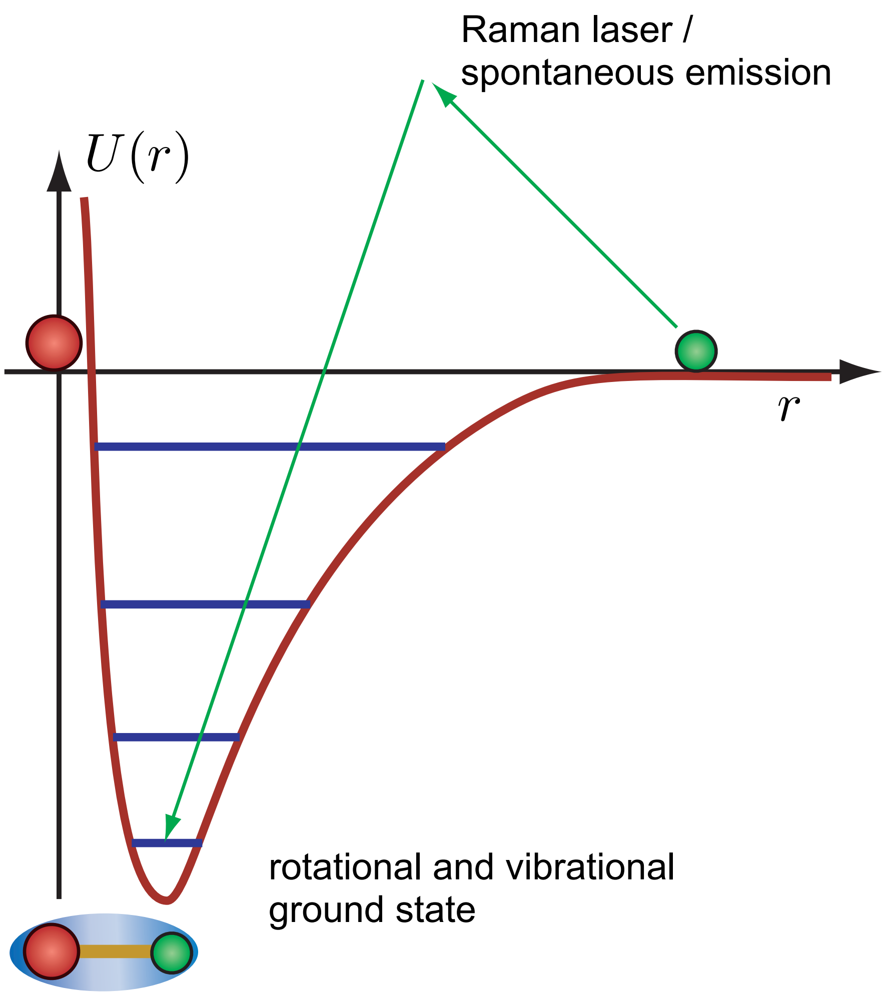
- Polar molecules in the rotational and vibrational ground state
- cooling and trapping techniques beeing developement:

  - cooling of polar molecules: e.g. stark decelerator

    D. DeMille, Yale
    J. Doyle, Harvard
    G. Rempe, Munich
    G. Meijer, Berlin
    J. Ye, JILA

  - photo association see J. Ye's talk (all cold atom labs)

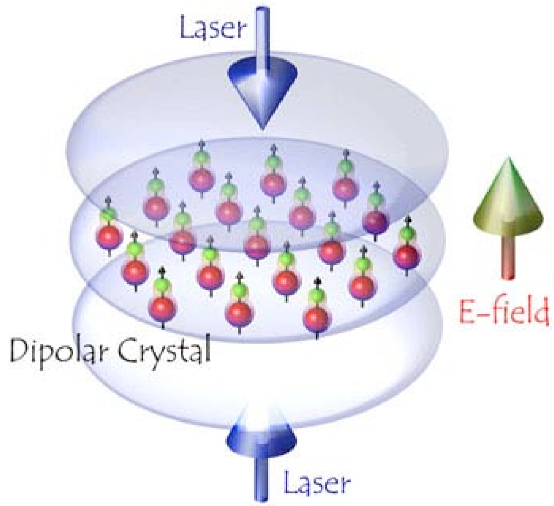
- bosonic molecules with closed electronic shell, e.g., SrO, RbCs, LiCs



Polar molecules

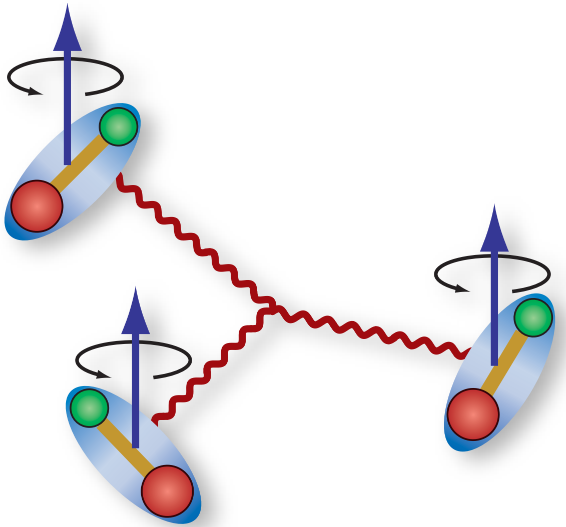
Crystalline phases

- long range dipole-dipole interaction
- interaction energy exceeds kinetic energy



Three-body interaction

- extended Hubbard models
- tunable three-body interaction



Polar molecule

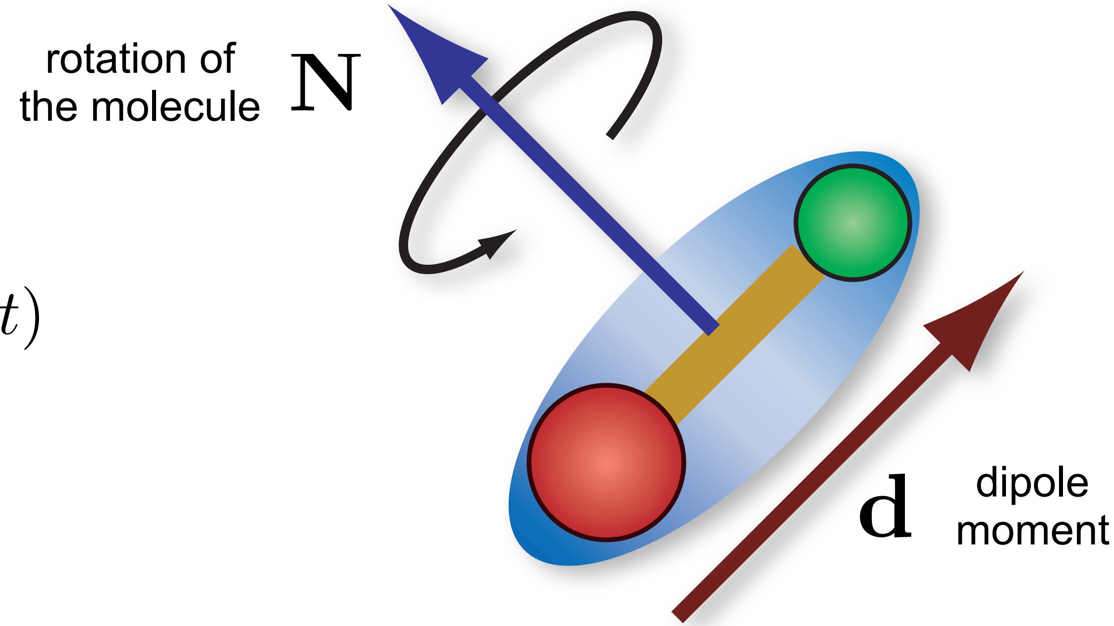
Low energy description

- rigid rotor in an electric field

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

$\mathbf{N}_i$: angular momentum

$\mathbf{d}_i$: dipole operator



$$BN_i(N_i+1)$$

$N=2$

$N=1$

$N=0$

$\sim 20\mathrm{GHz}$

Accessible via microwave

- anharmonic spectrum
- electric dipole transition

$$\Delta N = \pm 1 \qquad \Delta m_z = -1, 0, 1$$

- microwave transition frequencies
- no spontaneous emission

Interaction between polar molecules

Hamiltonian

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

kinetic energy	trapping potential	rigid rotor	electric field	interaction potential

Without external drive

- van der Waals attraction

$$V_{\rm vdW}(\mathbf{r}) = -\frac{C_6}{r^6}$$

$C_6 \approx d^4/6B$

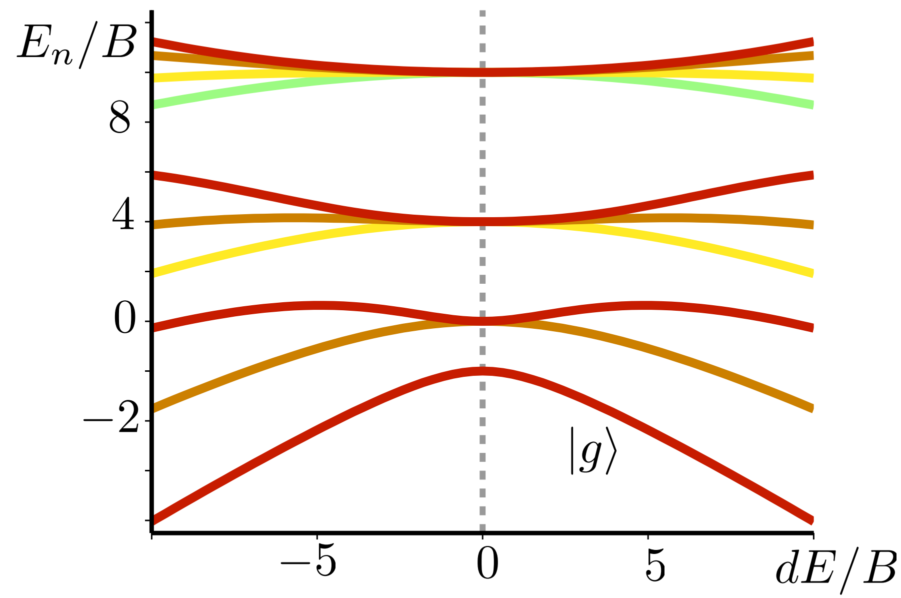
Static electric field

- internal Hamilton

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

- finite averaged dipole moment

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



Dipole-dipole interaction

Dipole-dipole interaction

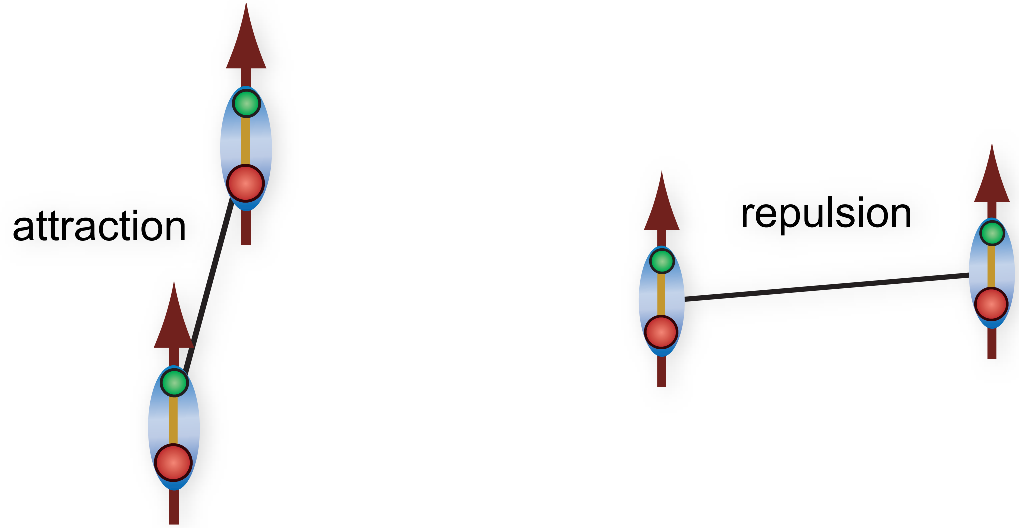
- anisotropic interaction
- long-range

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

- Born-Oppenheimer
  valid for:

$$r > R_{\text{rot}} = (D/B)^{1/3}$$

$$r > (Ed/D)^{1/3}$$

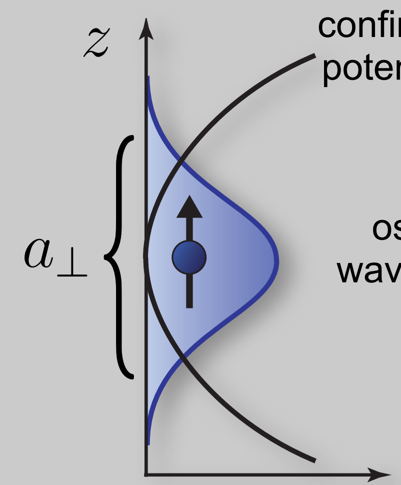


attraction → Instability in the many-body system

- collaps of the system for increasing dipole interaction $\frac{Dm}{\hbar^2 a_s} \gtrsim 1$
- roton softening
- supersolids?
  (Goral et. al. ‘02, L. Santos et al. ‘03, Shlyapnikov ‘06)

Stability:

- strong interactions
- confining into 2D by an optical lattice



Stability via transverse confining

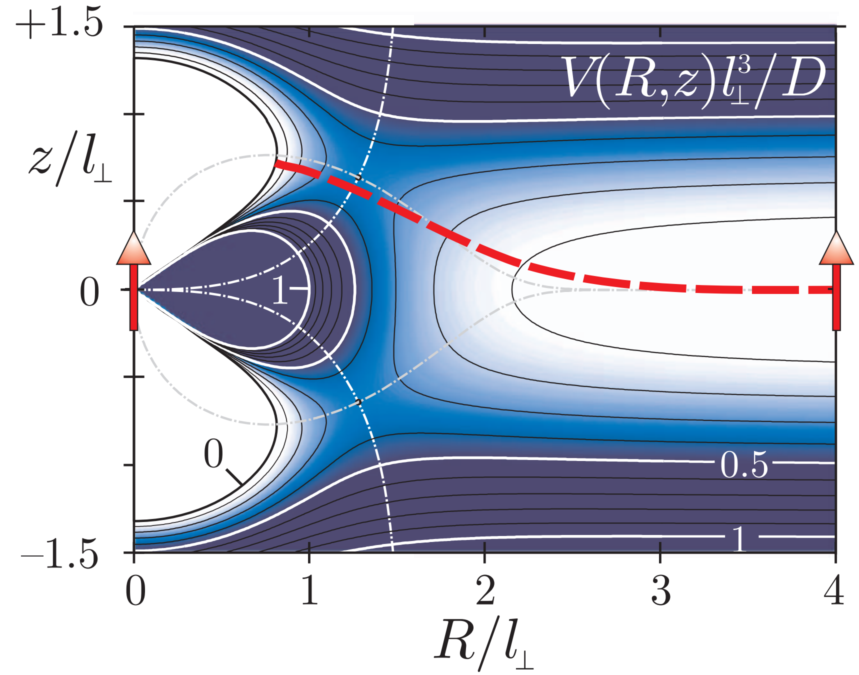
Effective interaction

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

- potential barrier: larger than kinetic energy



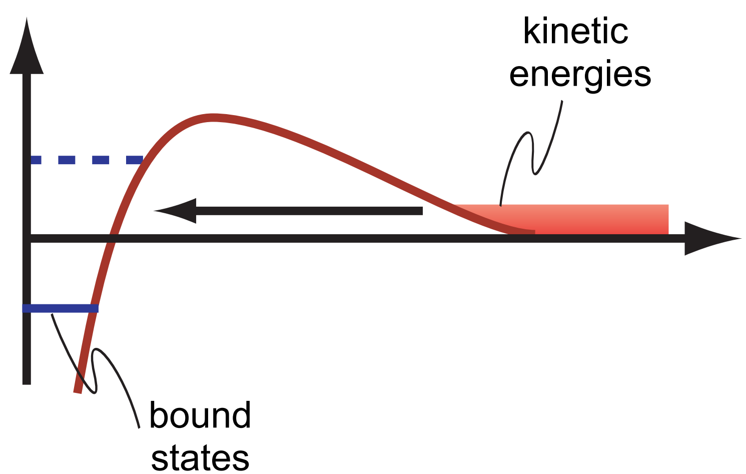
Tunneling rate:

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

attempt frequency

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

numerical factor: $\quad C \approx 5.8$



Crystalline phase

Hamiltonian

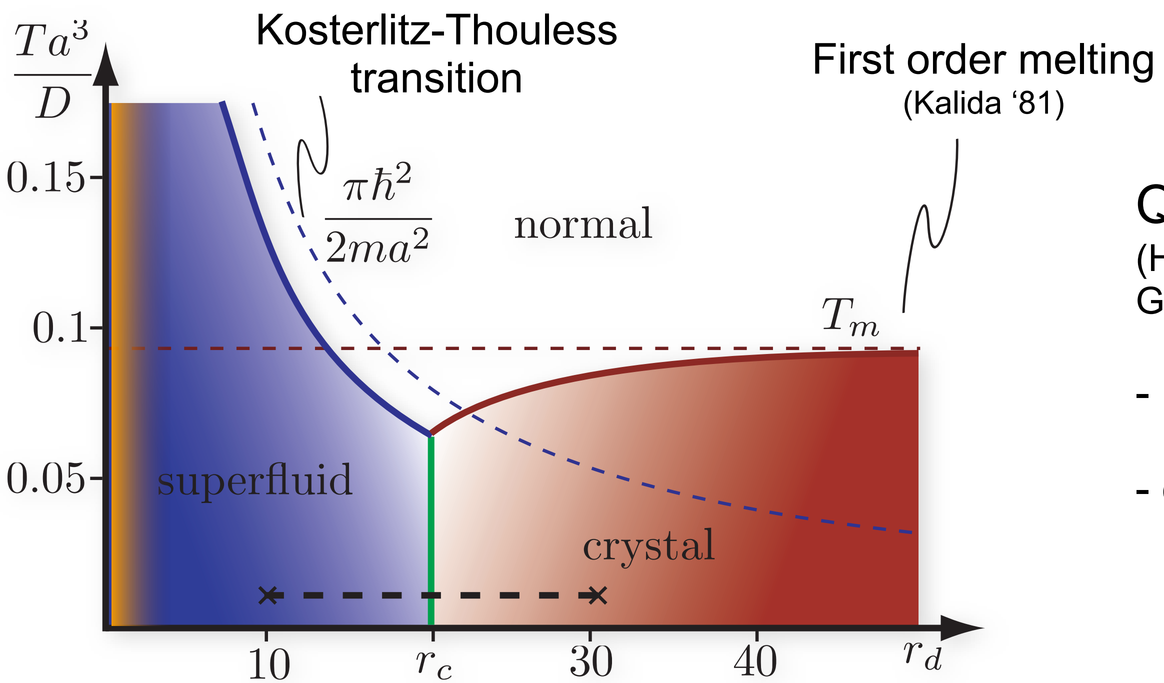
- polar molecules confined into a two-dimensional plane

interaction strength:

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

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

$$r_d = 1 - 300$$



Quantum melting

(H.P. Büchler, E. Demler, M. Lukin, A. Micheli, G. Pupillo, P. Zoller, PRL 2007)

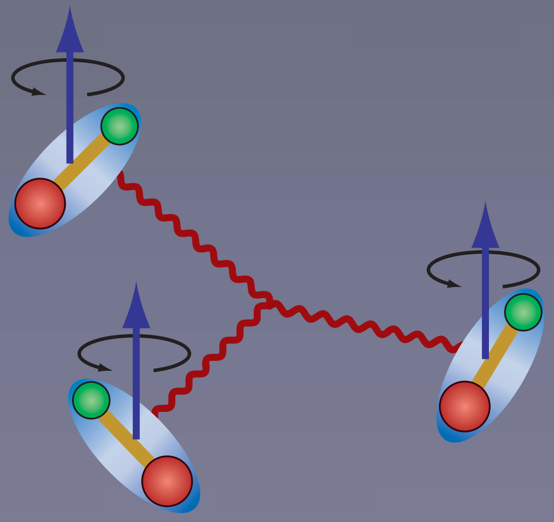
- indication of a first order transition

- critical interaction strength

$$r_d \approx 20$$

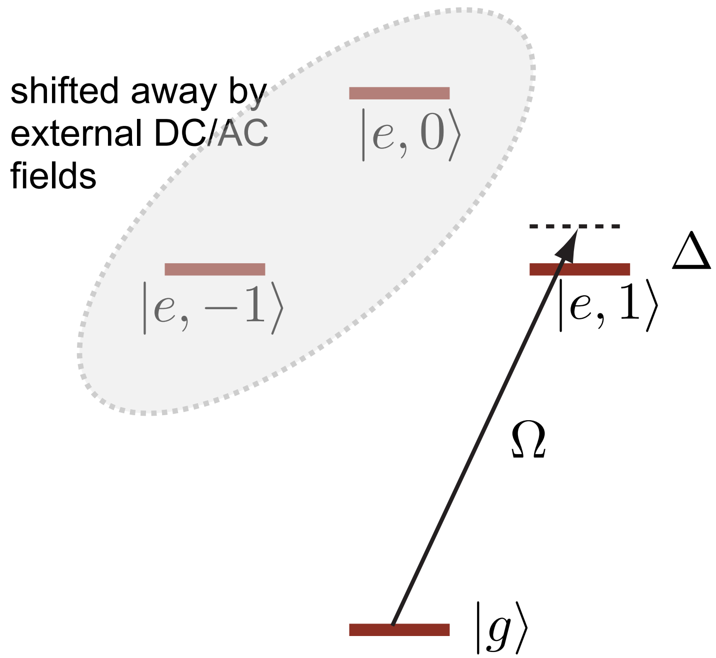
Three-body interactions

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



H.P. Büchler, A. Micheli, and P. Zoller
cond-mat/0703688 (2007).

Single polar molecule



Static electric field

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

$$d_g = \langle g|d_z|g\rangle$$

$$d_e = \langle e,1|d_z|e,1\rangle$$

Mircowave field

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

Δ : detuning
Ω : rabi frequency

- restrict to two states
- ignore influence of $|e,-1\rangle$
- rotating wave approximation

- anharmonic spectrum
- electric dipole transition

$$\Delta N = \pm 1 \qquad \Delta m_z = -1, 0, 1$$

- microwave transition frequencies
- no spontaneous emission

Many-body Hamiltonian

Many-body Hamiltonian

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_i V_{\mathrm{trap}}(\mathbf{r}_i) + \sum_i H_0^{(i)} + H_{\mathrm{int}}^{\mathrm{stat}} + H_{\mathrm{int}}^{\mathrm{ex}}$$

- external potentials:
  - trapping potential
  - optical lattices

- dipole-Dipole interaction
- restriction to the two internal states:

$$|g\rangle_i \quad |e,1\rangle_i$$

Two-level System

- rotating wave approximation

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

- two-level system in an effective magnetic field

- two 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

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

Dipole-dipole interaction

Microwave photon exchange

- $D = |\langle e, 1|\mathbf{d}|g\rangle|^2 \approx d^2/3$

$$H_{\text{int}}^{\text{ex}} = -\frac{1}{2}\sum_{i\neq j}\frac{D}{2}\nu(\mathbf{r}_i - \mathbf{r}_j)\left[S_i^+ S_j^- + S_j^+ S_i^-\right]$$

dipole-dipole interaction

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

Induced dipole moments

- $\eta_{d,g} = d_{e,g}/\sqrt{D}$

$P_i = |g\rangle\langle g|_i$

$$H_{\text{int}}^{\text{stat}} = \frac{1}{2}\sum_{i\neq j} D\nu\left(\mathbf{r}_i - \mathbf{r}_j\right)\left[\eta_g P_i + \eta_e Q_i\right]\left[\eta_g P_j + \eta_e Q_j\right]$$

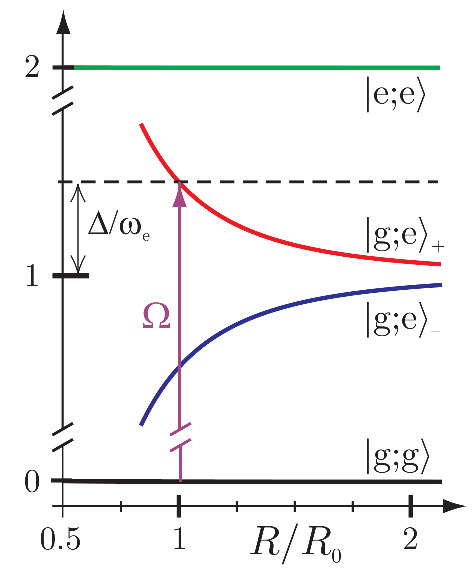
$Q_i = |e, 1\rangle\langle e, 1|_i$

Born-Oppenheimer potentials

Effective interaction

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

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



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

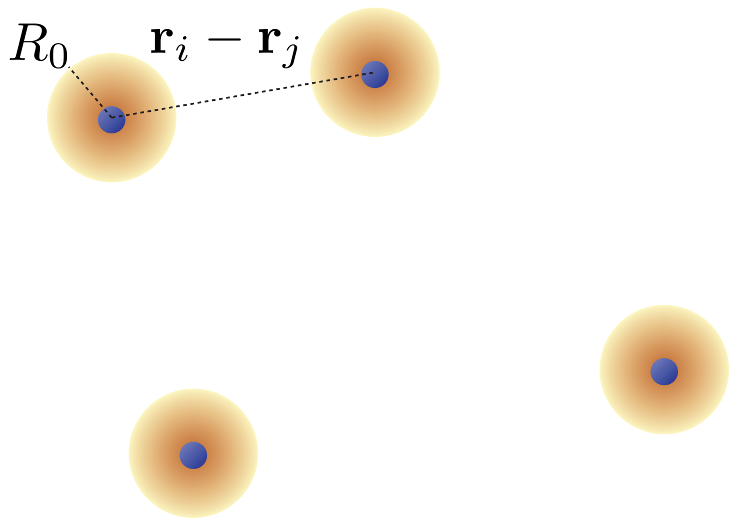
(iii) Adiabatically connected to the groundstate

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

"weak" dipole interaction

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

interparticle distance



Born-Oppenheimer potential

First order perturbation

- $E^{(1)}(\{\mathbf{r}_i\}) = \langle G | H_{\rm int}^{\rm ex} + H_{\rm int}^{\rm stat} | G \rangle$
- $|G\rangle = \prod_i \left(\alpha |g\rangle_i + \beta |e, 1\rangle_1\right)$

$$E^{(1)}(\{\mathbf{r}_i\}) = \frac{1}{2}\lambda_1 \sum_{i \neq j} D\nu(\mathbf{r}_i - \mathbf{r}_j)$$

dipole-dipole interaction: $V_{\rm eff}(\mathbf{r}) = \lambda_1 \frac{1 - 3\cos\theta}{r^3}$

Dimensionless coupling parameter

- $$\lambda_1 = \left(\alpha^2 \eta_g + \beta^2 \eta_e\right)^2 - \alpha^2 \beta^2$$

- tunable by the external electric field dE/B and the ratio Ω/Δ .

- for a magic rabi frequency the dipole-dipole interaction vanishes

$$\lambda_1 = 0$$

Born-Oppenheimer potential

Second order perturbation

$$E^{(2)}\left(\{\mathbf{r}_i\}\right) = \sum_{k\neq i\neq j} \frac{|M|^2}{\sqrt{\Delta^2+\Omega^2}} D^2 \nu\left(\mathbf{r}_i - \mathbf{r}_k\right) \nu\left(\mathbf{r}_j - \mathbf{r}_k\right)$$

: three-body interaction

$$+ \sum_{i\neq j} \frac{|N|^2}{\sqrt{\Delta^2+\Omega^2}} \left[D\nu\left(\mathbf{r}_i - \mathbf{r}_j\right)\right]^2$$

: repulsive two-body interaction

Matrix elements

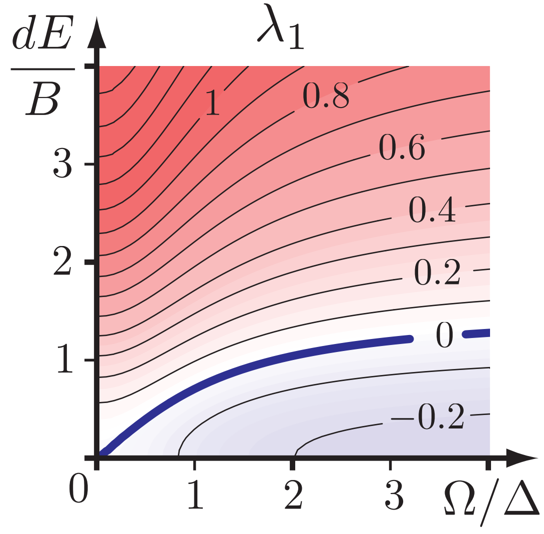
- $M = \alpha\beta\left[\left(\alpha^2\eta_g + \beta^2\eta_e\right)\left(\eta_e - \eta_g\right) + (\beta^2 - \alpha^2)/2\right]$

$$N = \alpha^2\beta^2\left[\left(\eta_e - \eta_g\right)^2 + 1\right]$$

Effective Hamiltonian

Effective interaction

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



- two-body interaction

$$V(\mathbf{r}) = \lambda_1 D\,\nu\left(\mathbf{r}\right) + \lambda_2 D R_0^3\;\left[\nu\left(\mathbf{r}\right)\right]^2$$

- three-body interaction

$$W\left(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3\right) = \gamma_2 R_0^3 D\left[\nu(\mathbf{r}_{12})\nu(\mathbf{r}_{13}) + \nu(\mathbf{r}_{12})\nu(\mathbf{r}_{23}) + \nu(\mathbf{r}_{13})\nu(\mathbf{r}_{23})\right]$$

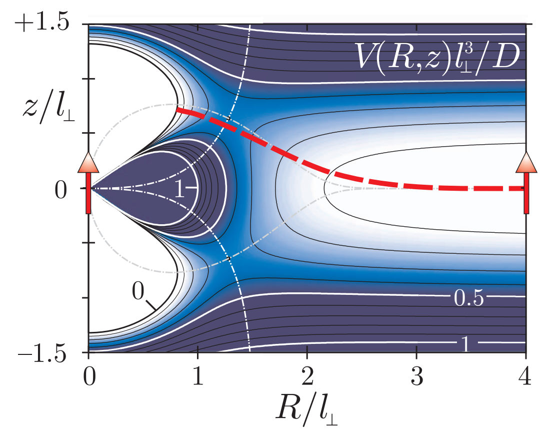
- validity is restricted to

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

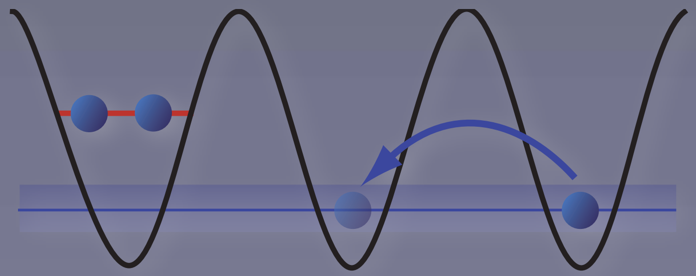
interparticle distance

(i) transverse confining into 2D

(ii) vanishing dipole-dipole interaction



Bose-Hubbard model

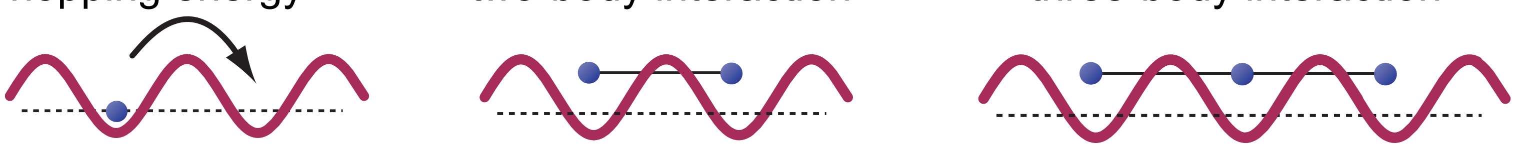


Hubbard model

Extended Bose-Hubbard models

- hardcore bosons

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



- interaction parameters for strong optical lattices

$$U_{ij} = V(\mathbf{R}_i - \mathbf{R}_j) \qquad W_{ijk} = W(\mathbf{R}_i, \mathbf{R}_j, \mathbf{R}_k)$$

Polar molecule: LiCs:

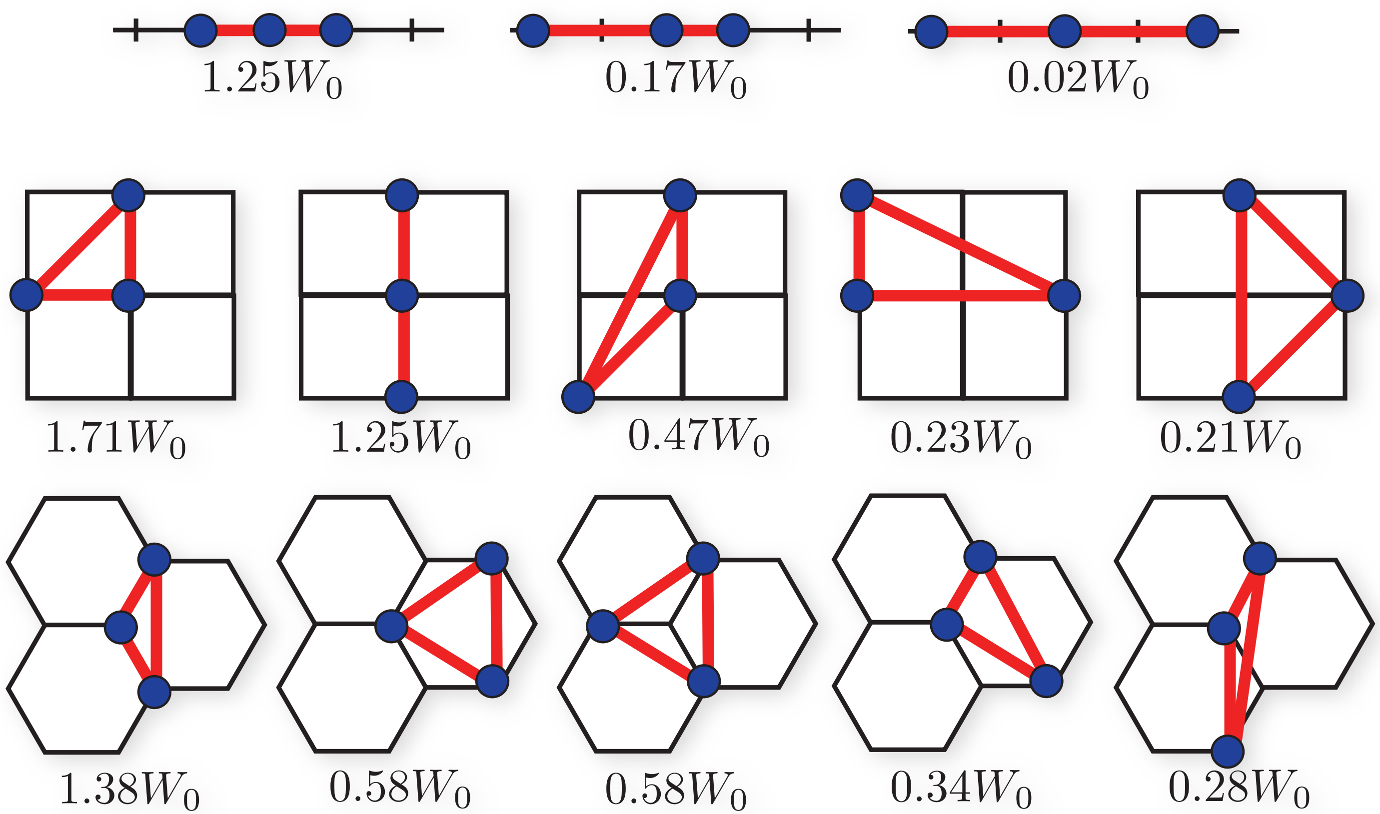
- dipole moment
  $d \approx 6\text{Debye}$
- hopping energy
  $J/E_r \sim 0 - 0.5$
- lattice spacing:
  $\lambda \approx 1000\,\text{nm}$
  $E_r \approx 1.4\,\text{kHz}$
- nearest neighbor interaction:
  $U/E_r \sim 30$
  $W/E_r \sim 30\,(R_0/a_{\rm L})^3$

Hubbard model

Three-body interaction

- next-nearest neighbor terms

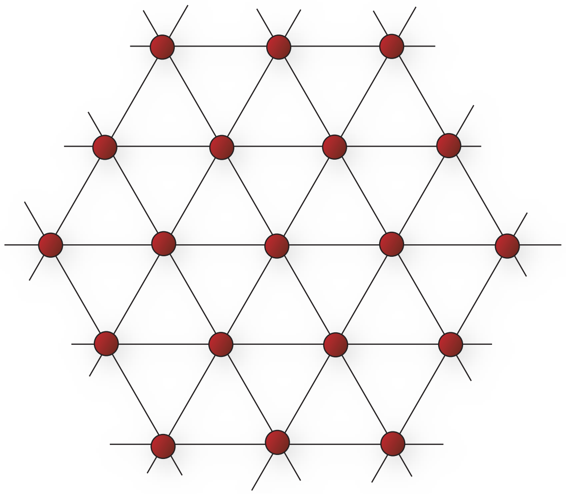
$$W_{ijk} = W_0 \left[\frac{a^6}{|\mathbf{R}_i - \mathbf{R}_j|^3 |\mathbf{R}_i - \mathbf{R}_k|^3} + perm \right]$$



Supersolids on a triangular lattice

$$H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{1}{2} \sum_{i \neq j \rangle} U_{ij} n_i n_j$$

$$U_{ij} \sim \frac{1}{|i-j|^3}$$: static electric field



Quantum Monte Carlo simulations

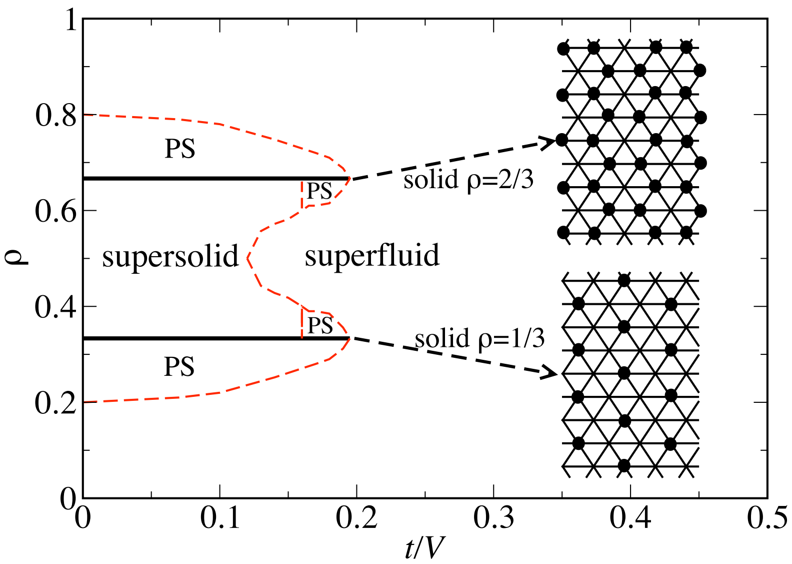
Wessel and Troyer, PRL (2005)
Melko *et al.*, PRB, (2006)

- supersolid close to half filling and strong nearest neighbor interactions

$$n = 1/2$$

$$U/J \gtrsim 10$$

- stable under next-nearest neighbor interactions



One-dimensional model

next-nearest neighbor interactions

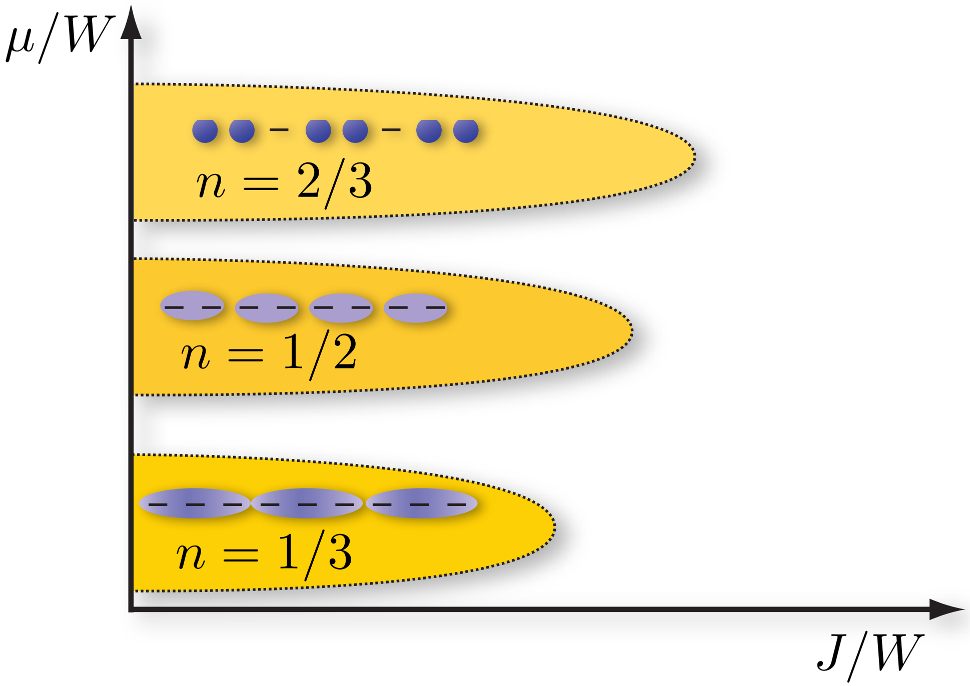
$$H = -J \sum_i b_i^\dagger b_{i+1} + W \sum_i n_{i-1} n_i \, n_{i+1} - \mu \sum_i n_i \quad + H_{\text{n.n.n.}}$$

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

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

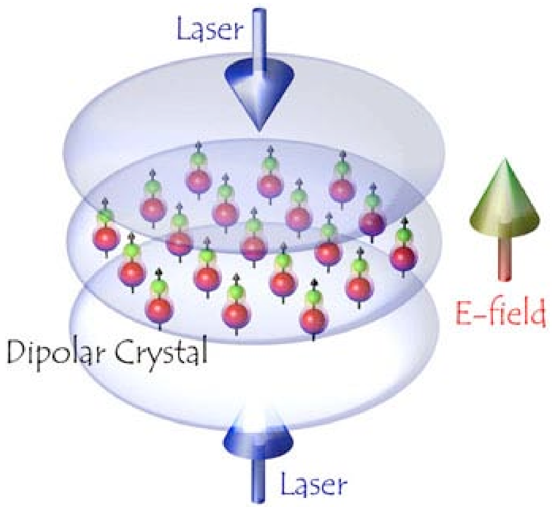
- hopping correlations (1D VBS)

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

Conclusion and Outlook

Polar molecular crystal

- reduced three-body collisions
- strong coupling to cavity QED
- ideal quantum storage devices

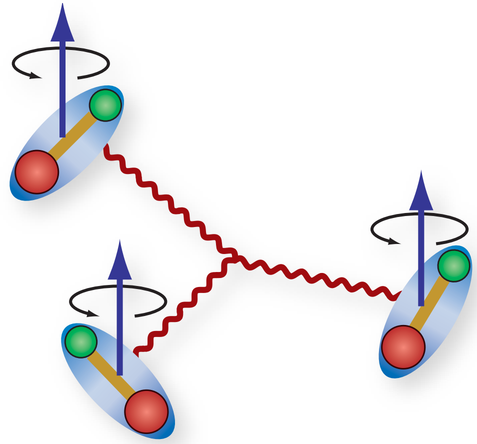


Lattice structure

- alternative to optical lattices
- tunable lattice parameters
- strong phonon coupling: polarons

Extended Hubbard models

- strong nearest neighbor interaction
- three-body interaction



Novel quantum matter

- supersolid phases
- string nets?