Hubbard Models with Molecules in Optical Lattices: Engineering three-body interactions

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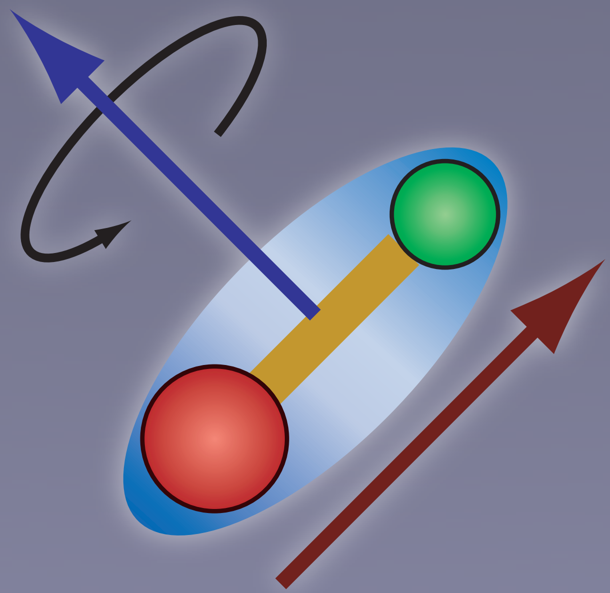


Atomic and molecular gases

Bose-Einstein condensation

- Gross-Pitaevskii equation
- non-linear dynamics

Quantum degenerate *dilute* atomic/molecular gases of fermions and bosons

control and tunability

Rotating condensates

- vortices
- fractional quantum Hall

Molecules

- Feshbach resonances
- BCS-BEC crossover
- polar molecules

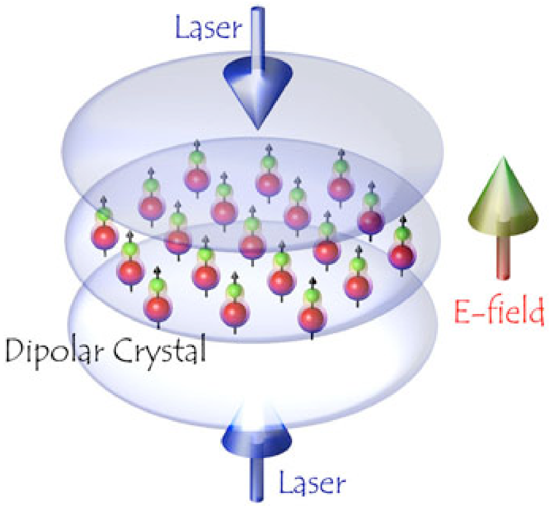
Optical lattices

- Hubbard models
- strong correlations
- exotic phases

Polar molecules

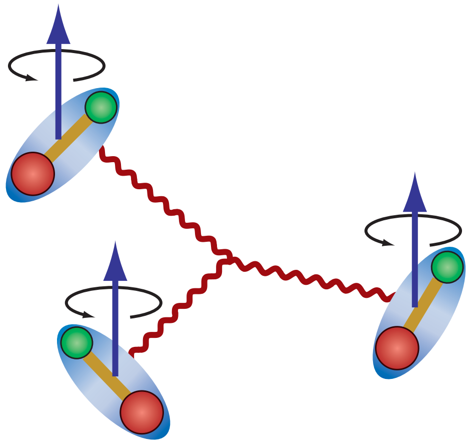
Crystalline phases

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



Three-body interaction

- tunable three-body interaction
- extended Hubbard models in the presence of optical lattices



Polar molecules

Why polar molecules?

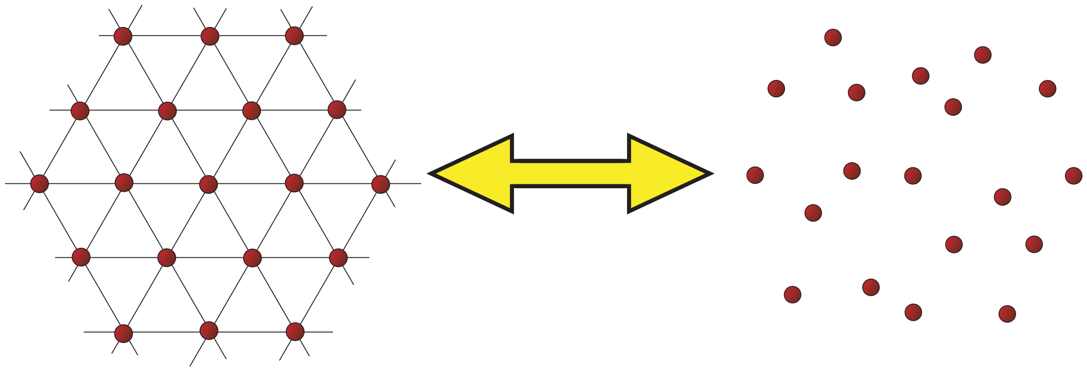
- coupling to optical and microwave fields
  - trapping/cooling
  - internal states
- permanent dipole moment
  - strong dipole-dipole interaction
  - long-range interaction

Polar molecules in 2D

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

Quantum melting

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



Polar molecules

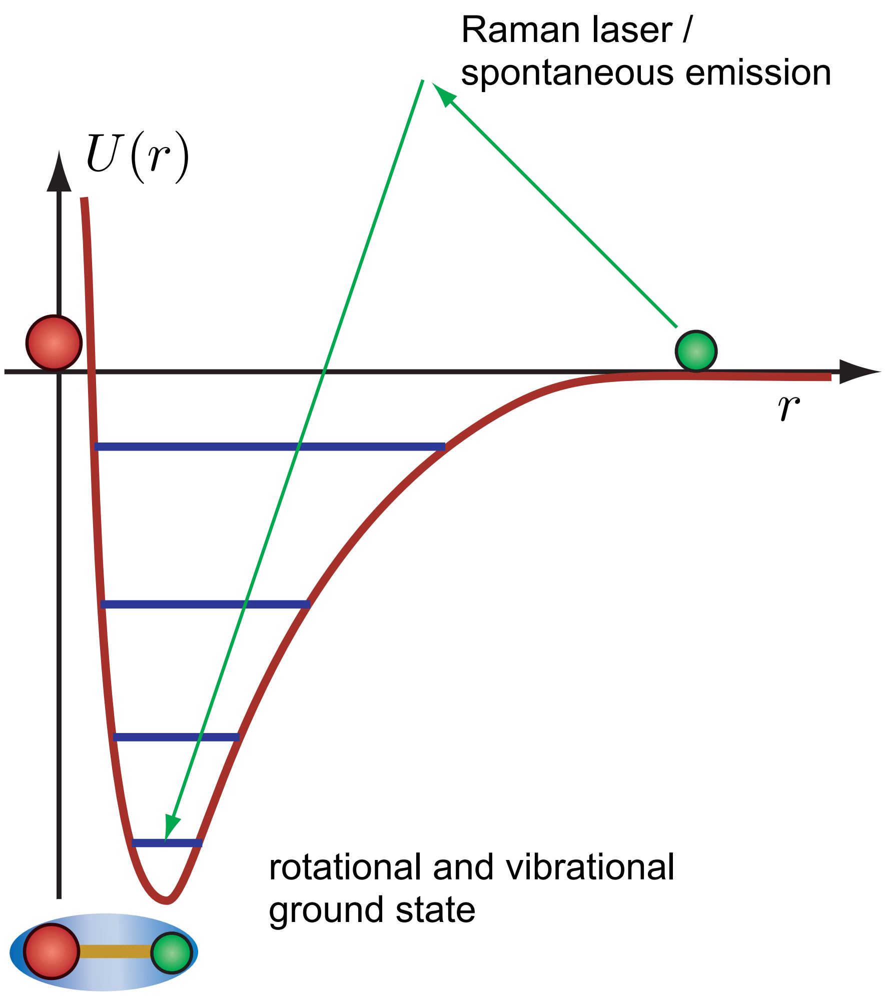
Experimental status

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

    - cooling of polar molecules:
      D. De Mille, Yale
      J. Doyle, Harvard
      G. Rempe, Munich
      G. Meijer, Berlin

    - photo association
      (all cold atom labs)

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



Polar molecule

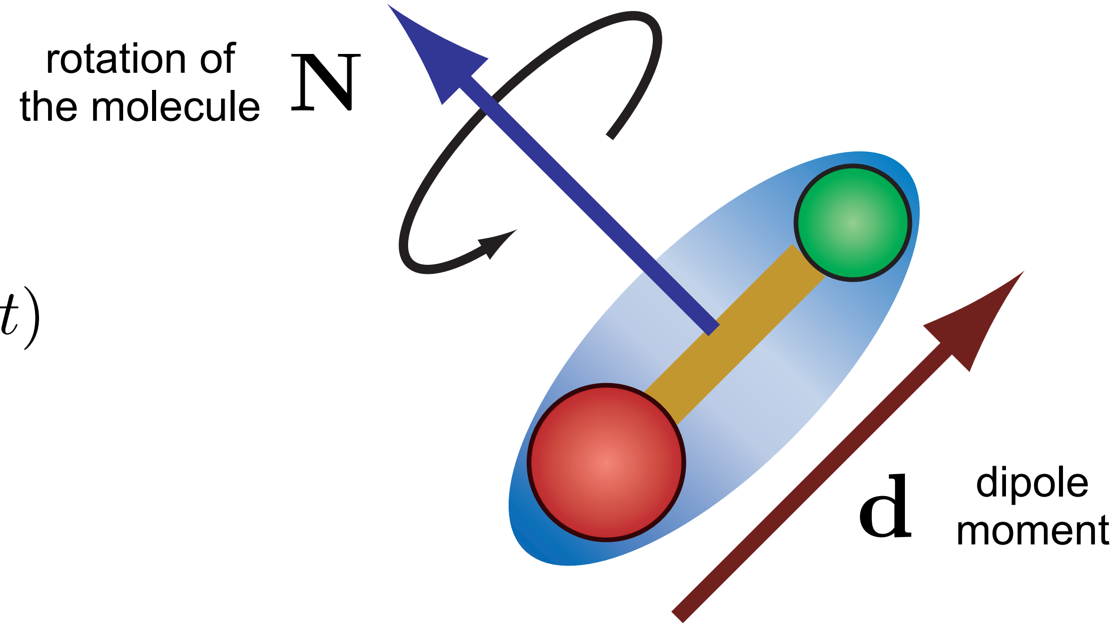
Low energy description

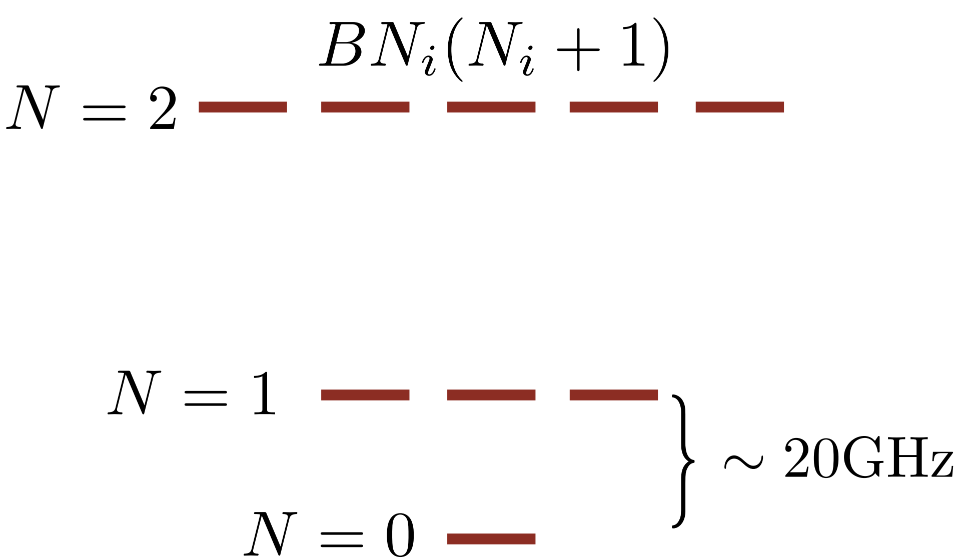
- rigid rotor in an electric field

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

$\mathbf{N}_i$: angular momentum

$\mathbf{d}_i$: dipole operator





Accessible via microwave

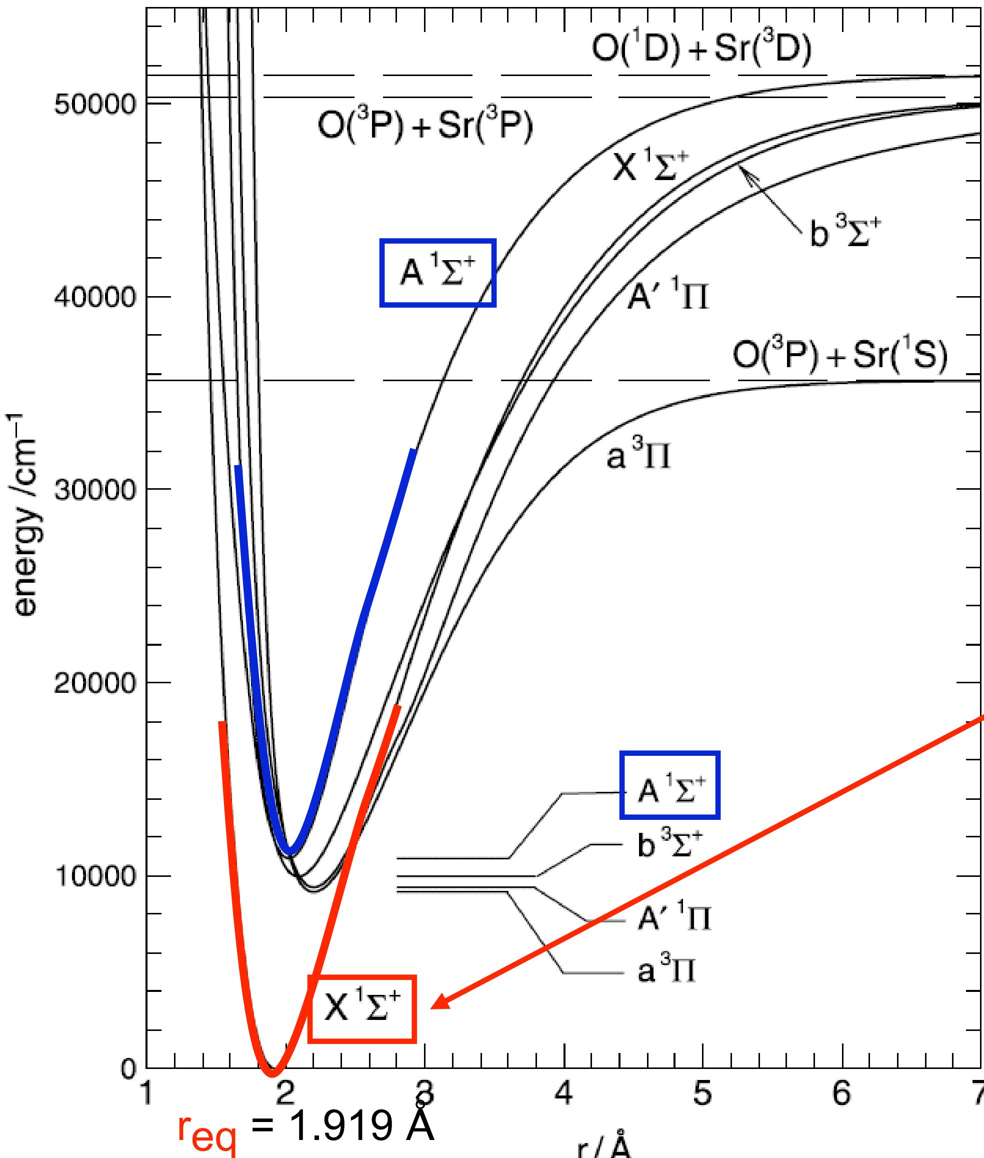
- anharmonic spectrum
- electric dipole transition

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

- microwave transition frequencies
- no spontaneous emission

Polar molecule

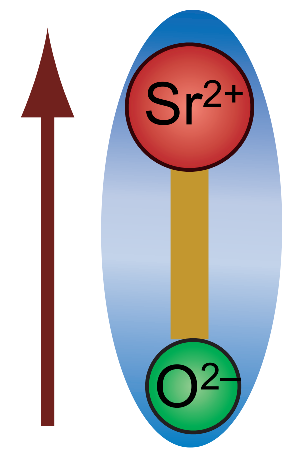
Rydberg-Klein-Rees (RKR)-potentials
(R. Skelton *et al.*, 2003)



r_{eq} = 1.919 Å
d = 8.9 D

heteronuclear molecule with strong persistent dipole moment in electronic groundstate.

$Sr^{2+}O^{2-}$ ... ionic binding



$_{38}$Sr	[Kr]$5s^2$	
^{88}Sr	$I^p = 0^+$	(83%)
^{86}Sr	$I^p = 0^+$	(10%)
^{87}Sr	$I^p = \frac{3}{2}^+$	(7%)

$_{8}$O	$1s2s^2p^4$	
^{16}O	$I^p = 0^+$	(99.76%)
^{18}O	$I^p = 0^+$	(0.20%)

$X\,^1\Sigma^+$ ... electronic groundstate:

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

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

ω_{eq} = 19.586 THz ... vibrational const.
B_{eq} = 10.145 GHz ... rotational
I=0 ... no nuclear momenta for ^{88}SrO, ^{86}SrO

Interaction between 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

Without external drive

- van der Waals attraction

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

$C_6 \approx d^4/6B$

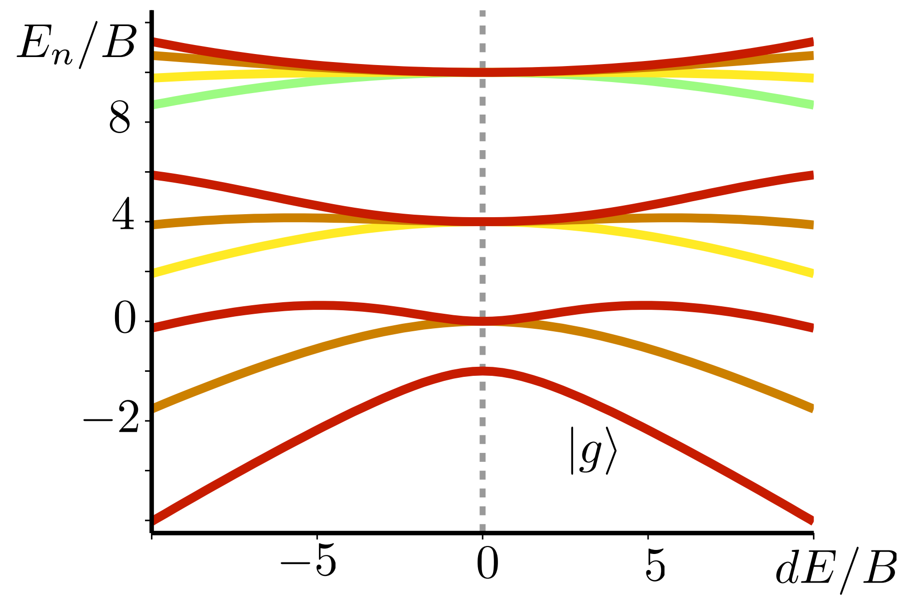
Static electric field

- internal Hamilton

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

- finite averaged dipole moment

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



Dipole-dipole interaction

Dipole-dipole interaction

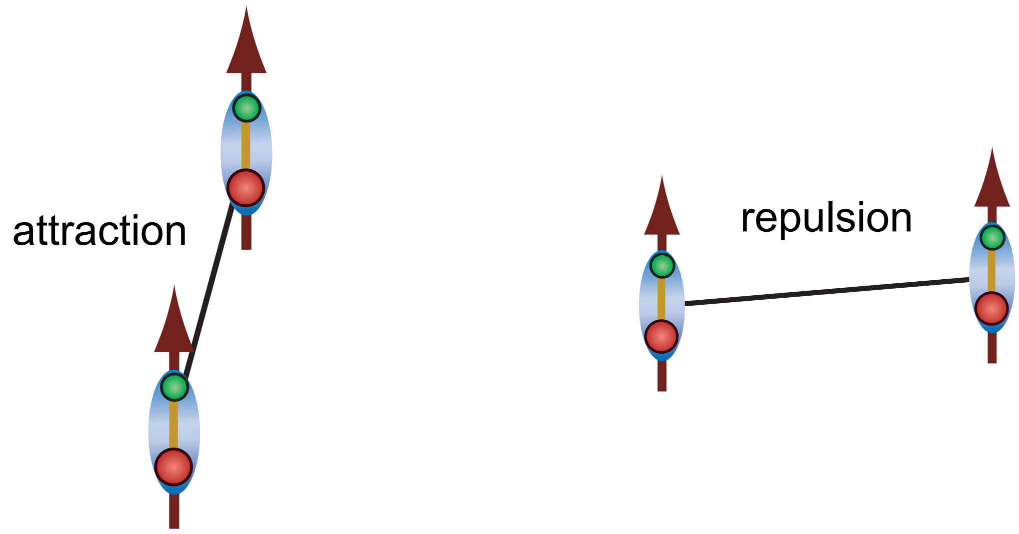
- anisotropic interaction
- long-range

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

- Born-Oppenheimer valid for:

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

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



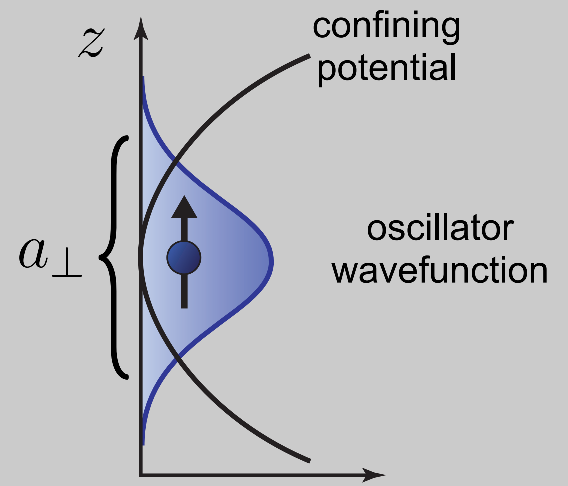
attraction → Instability in the many-body system

- 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

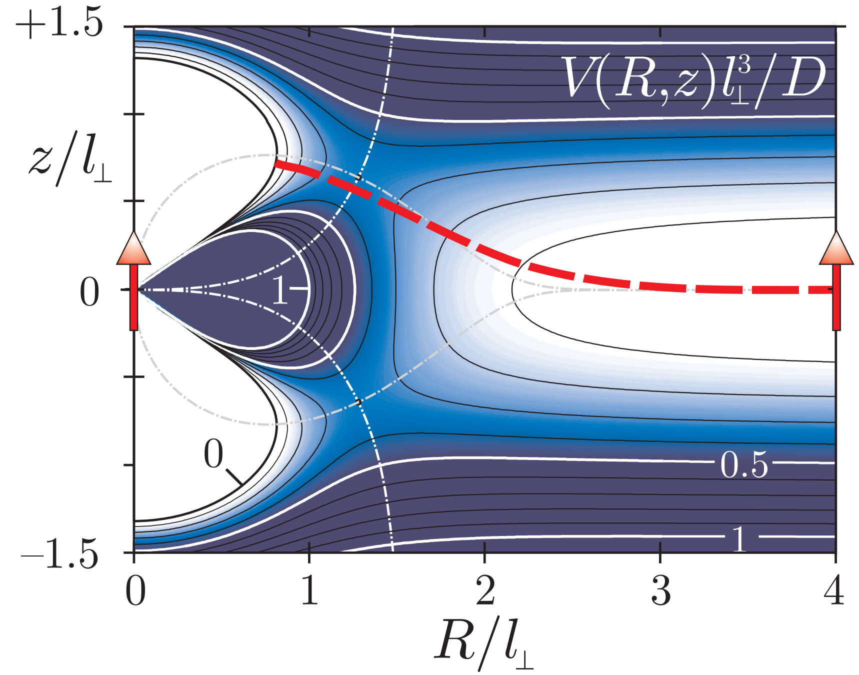
- interaction potential with transverse trapping potential

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

- characteristic length scale

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

- potential barrier: larger than kinetic energy



Tunneling rate:

- semi-classical rate (instanton techniques)

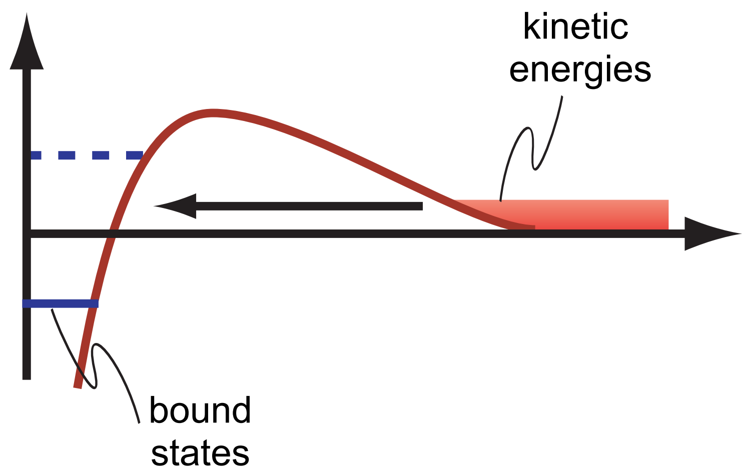
$$\Gamma = A\exp\left(-S_E/\hbar\right)$$

attempt frequency

- Euclidean action of the instanton trajectory

$$S_E = \hbar\left(\frac{Dm}{\hbar^2 a_\perp}\right)^{2/5} C$$

numerical factor: $C \approx 5.8$



Static electric field

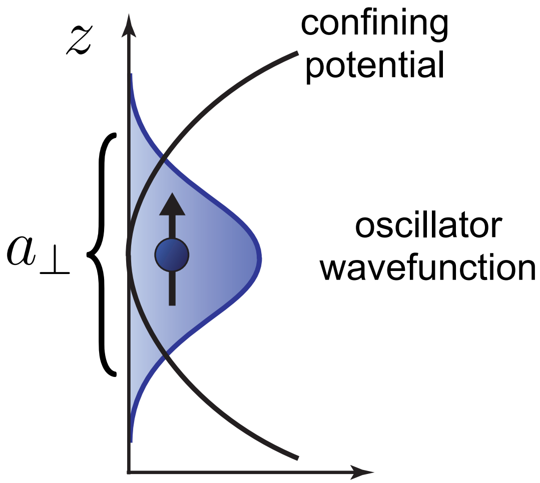
Transverse trapping

- integrating out the fast transverse motion of the molecules

transverse wave function

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

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

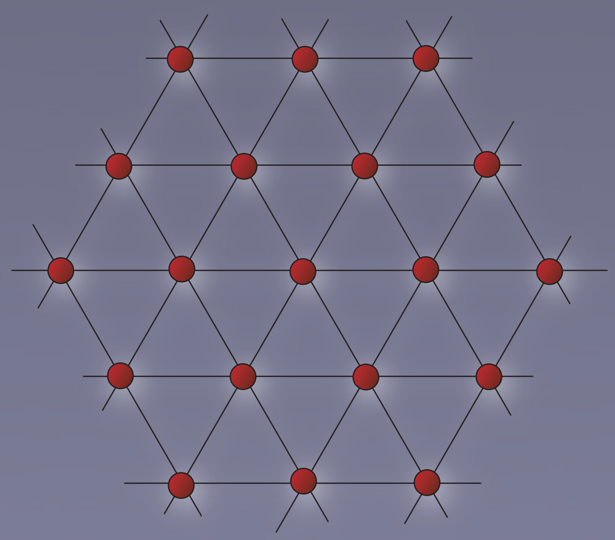


Effective 2D potential

- large distances $|\mathbf{R}| > l_\perp$

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

Crystalline phase



Effective Hamiltonian

Hamiltonian

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

interaction strength: $r_s = \frac{E_{\text{int}}}{E_{\text{kin}}} = \frac{Dm}{\hbar^2 a}$

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

Polar molecule: SrO

- dipole moment:

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

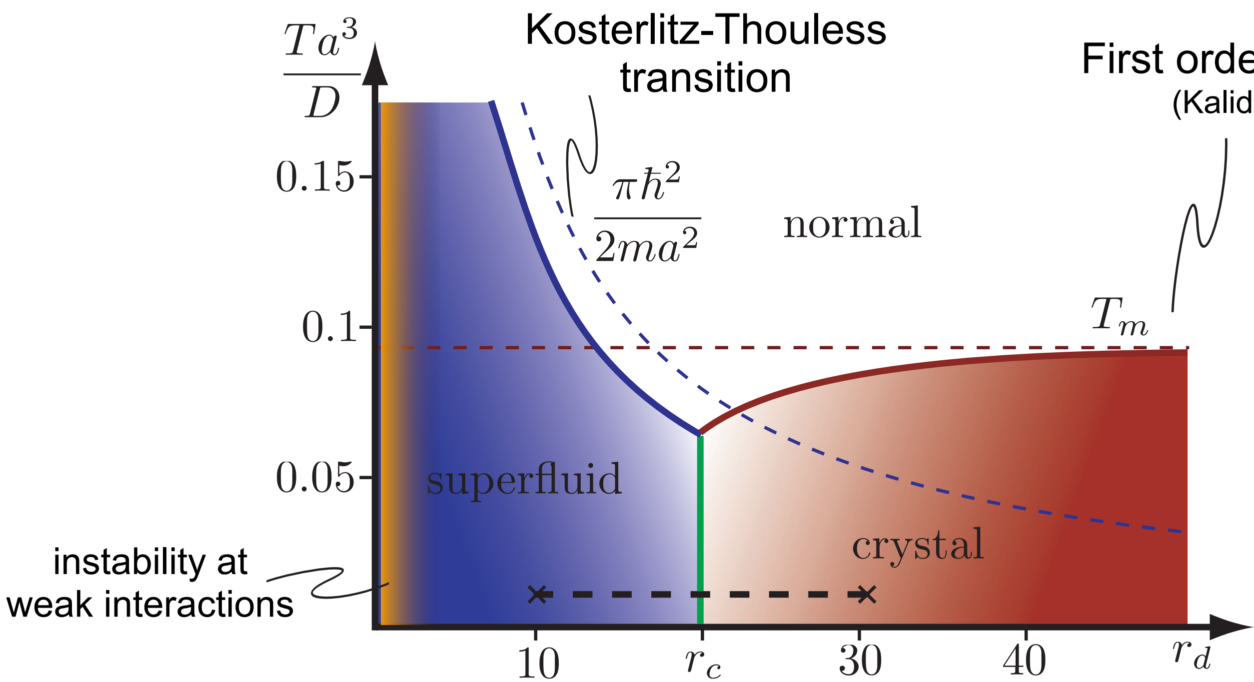
$$r_s \sim 121 \mu m / a$$

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

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

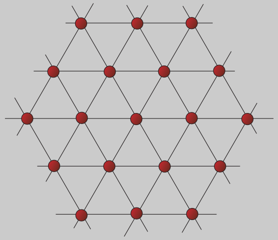
- stability: $S_{\text{E}}/\hbar \gtrsim 130$

Quantum Phase transition



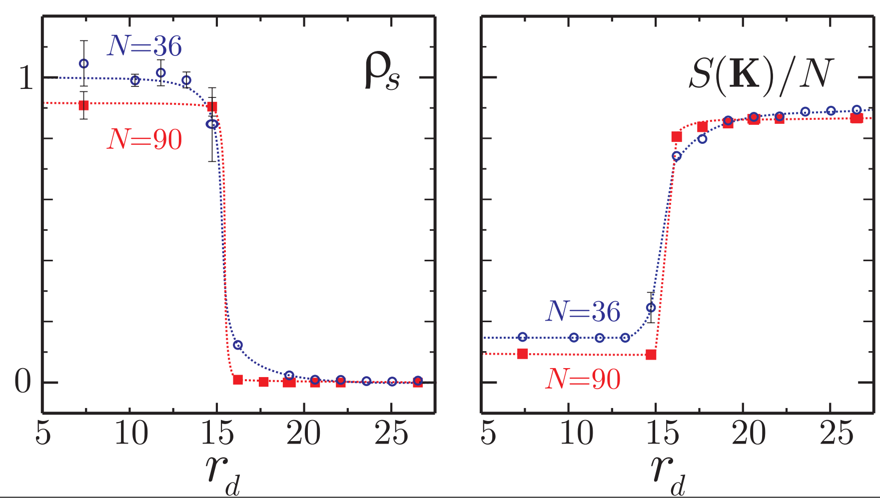
Crystal phase

- triangular lattice structure
- phonon modes



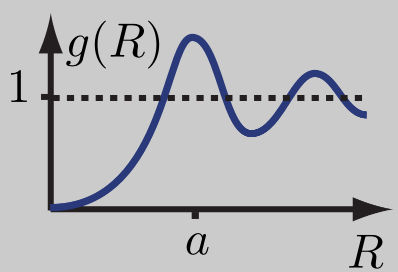
Quantum melting

- indication of a first order transition
- Quantum Monte Carlo simulations

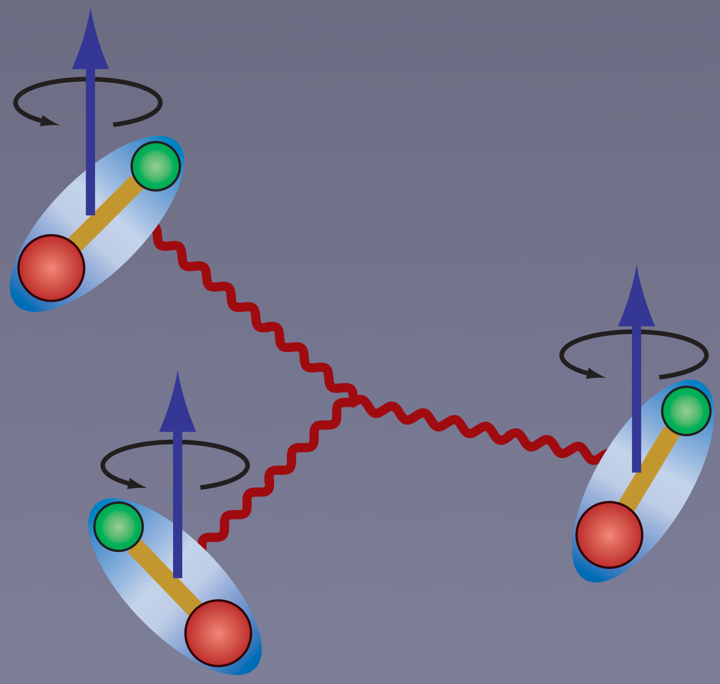


Strongly interacting superfluid

- superfluid stiffness
- large depletion



Three-body interactions



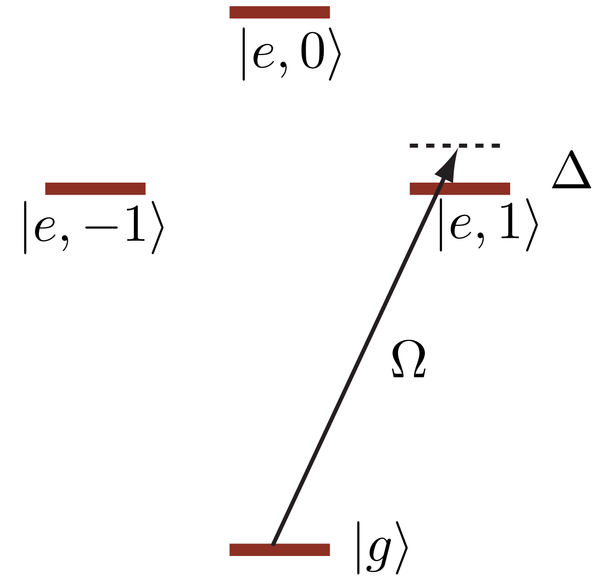
Single polar molecule

Static electric field

- along the z-axes
- splitting the degeneracy of the first excited states
- 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.

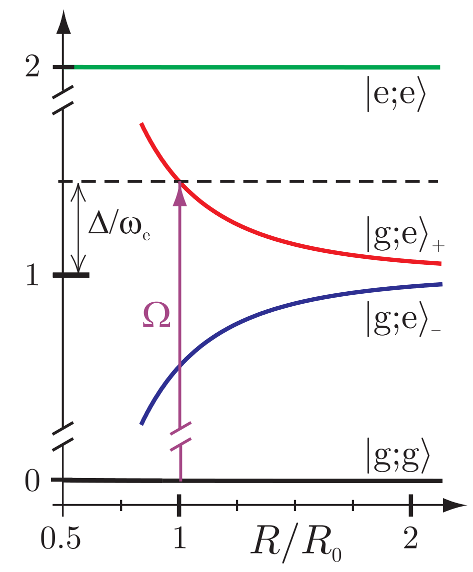
(iii) Adiabatically connected to the groundstate

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

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

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

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

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

- special point

$$\lambda_1 = 0$$
$$M = 0$$

→ repulsive two-body interaction

Effective Hamiltonian

Effective interaction

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

- 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

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

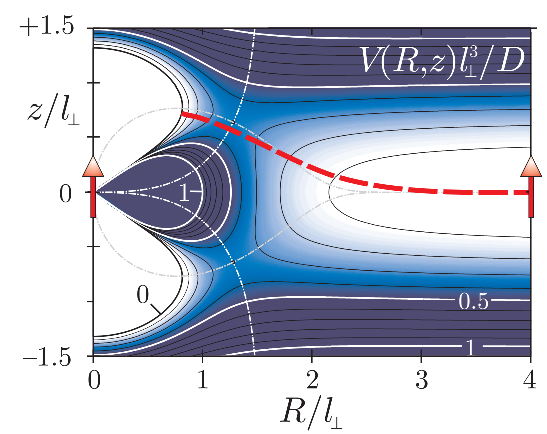
- validity is restricted to

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

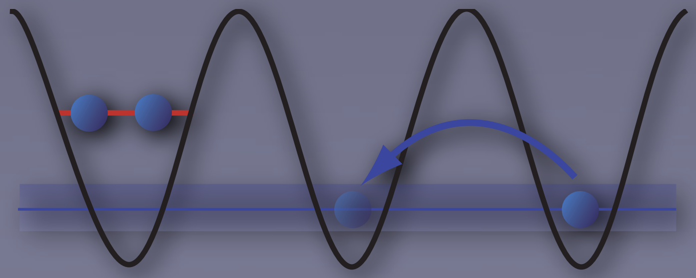
interparticle distance

(i) transverse confining into 2D

(ii) vanishing dipole-dipole interaction



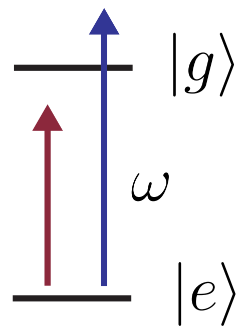
Bose-Hubbard model

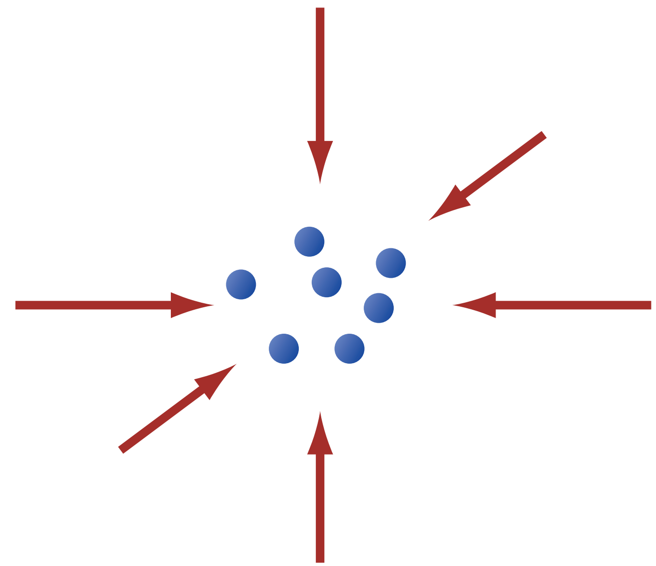


Optical lattices

- AC Stark shift

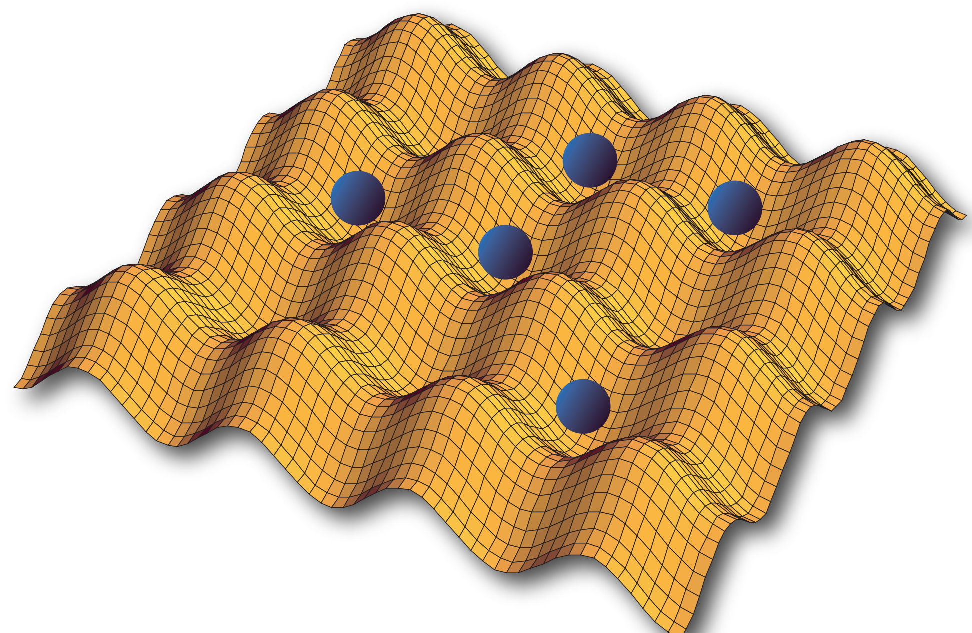
off-resonant
laser





- periodic potentials

$$V(\mathbf{x}) = V_0 \sin^2 \mathbf{k}\,\mathbf{x} + \ldots$$



- 2D and 1D setups
- different lattice structures

- characteristic energies

$$E_{\mathrm{r}} = \frac{\hbar^2 \mathbf{k}^2}{2m} \sim 10\mathrm{kHz}$$

$$V_0 / E_{\mathrm{r}} \sim 50$$

Microscopic Hamiltonian

$$H = \int d\mathbf{x} \psi^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\Delta + V_{\rm trap}(\mathbf{x}) \right) \psi(\mathbf{x}) + H_{\rm int}$$

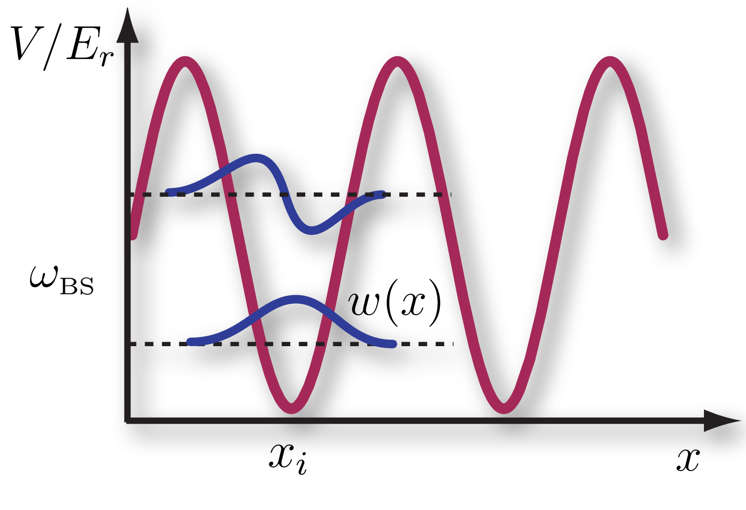
optical lattice

effective interaction $V_{\rm eff}$

- strong opitcal lattice $V > E_{\rm r}$
- express the bosonic field operator in terms of Wannier functions
- restriction to lowest Bloch band

Jaksch *et al,* PRL (1998)

$$\psi(\mathbf{x}) = \sum_i w(\mathbf{x} - \mathbf{x}_i) b_i$$



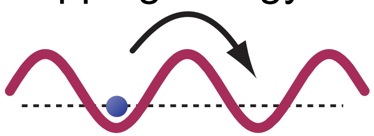
Hubbard model

Extended Bose-Hubbard models

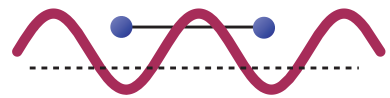
- hardcore bosons

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

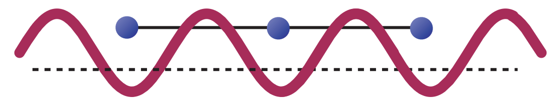
hopping energy



two-body interaction



three-body interaction



- 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

  $d \approx 6\mathrm{Debye}$

- hopping energy

  $J/E_r \sim 0 - 0.5$

- lattice spacing: $\lambda \approx 1000\,\mathrm{nm}$, $E_r \approx 1.4\,\mathrm{kHz}$

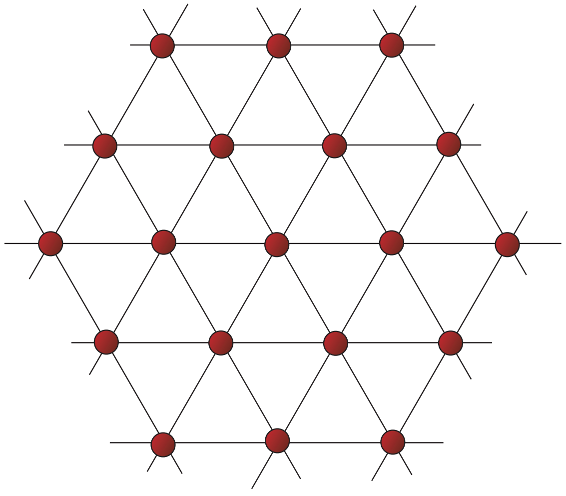
- nearest neighbor interaction: $U/E_r \sim 30$, $W/E_r \sim 30\,(R_0/a_{\mathrm{L}})^3$

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

$$U_{ij} \sim \frac{1}{|i-j|^6}$$: static electric field + microwave field



Quantum Monte Carlo simulations

Wessel and Troyer, PRL (2005)

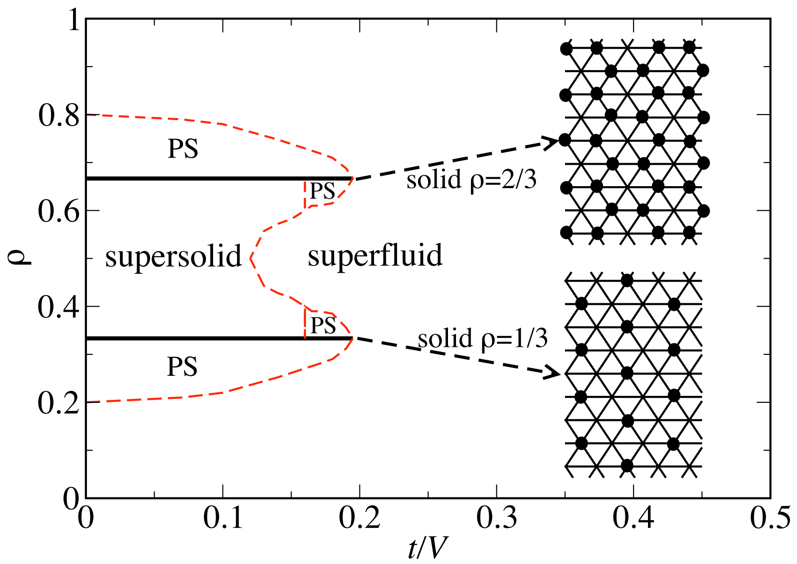
Melko *et al.*, PRB, (2006)

- 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

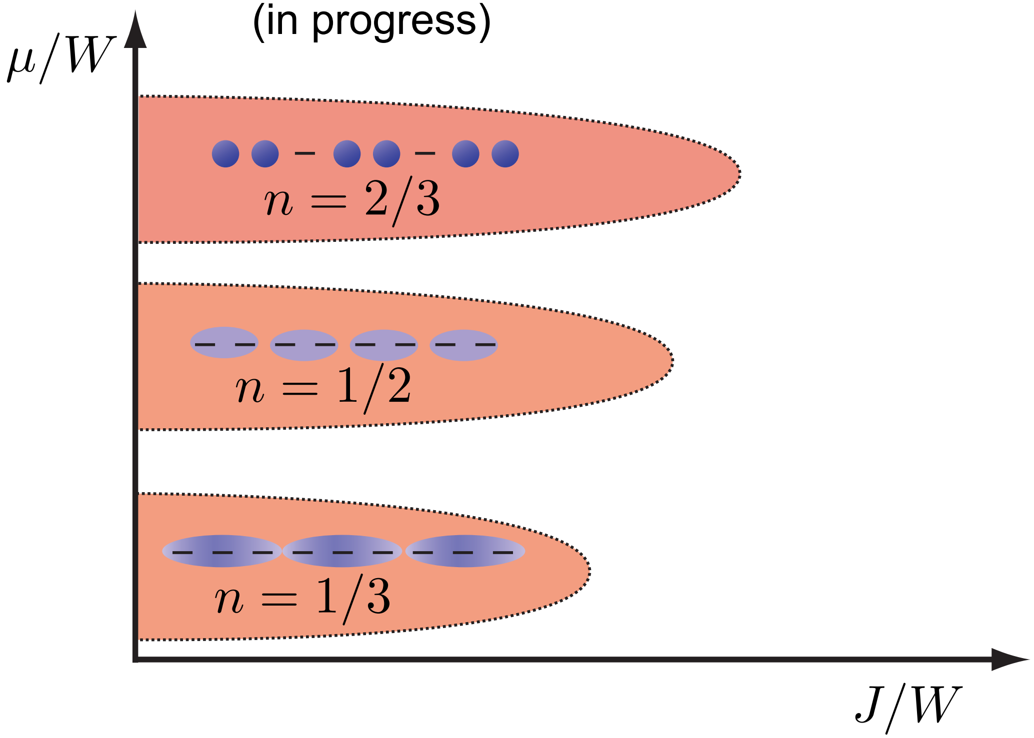
$$H = -J\sum_i b_i^\dagger b_{i+1} + W\sum_i n_{i-1}n_i\, n_{i+1} - \mu\sum_i n_i \quad + H_{\text{n.n.n.}}$$

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)

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

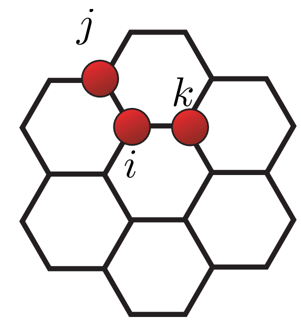
String nets

Honeycomb lattice

- interaction Hamiltonian

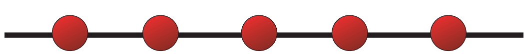
$$H_{\text{int}} = W \sum_{\langle\langle ijk \rangle\rangle} n_i n_j \, n_k \quad + H_{\text{n.n.n.}}$$

next-nearest neighbor interactions

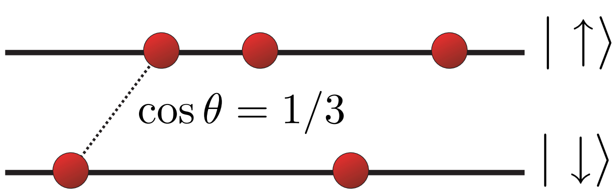


- integer filling within a single layer
- split the layer into a double layer

maps to an effective spin system



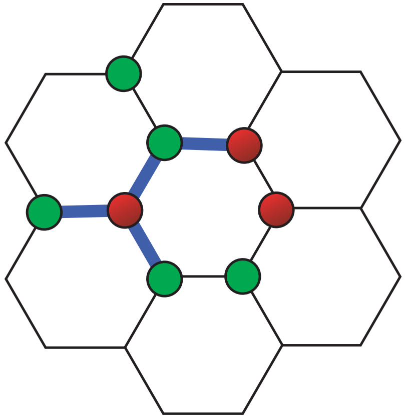
each well splits into a double well



Spin-Hamiltonian

$$H_{\text{spin}} = W \sum_{\langle\langle ijk \rangle\rangle} P_{S_{\text{tot}}=\pm 3/2}$$

- penalizes three successive spins
- allowed configurations are characterized by string nets (Fidkowski, *et al*, 2006)

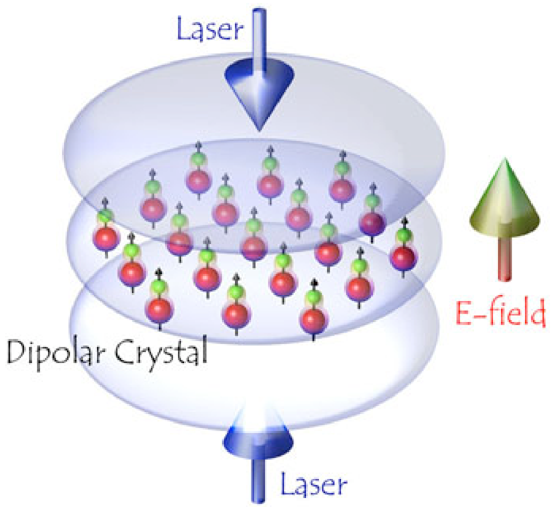


Next-nearest neighbor interactions?

Conclusion and Outlook

Polar molecular crystal

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

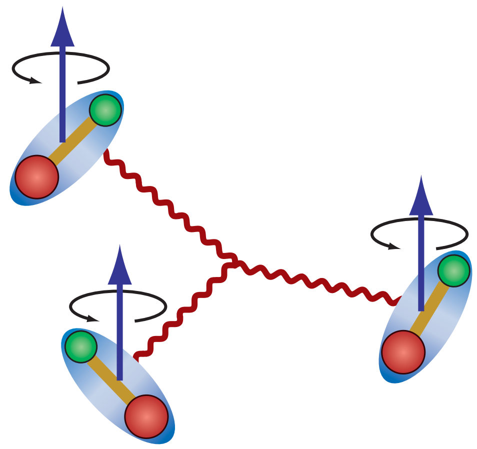


Lattice structure

- 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?