Phases diagrams of ultra-cold dipolar Bosons

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Outline

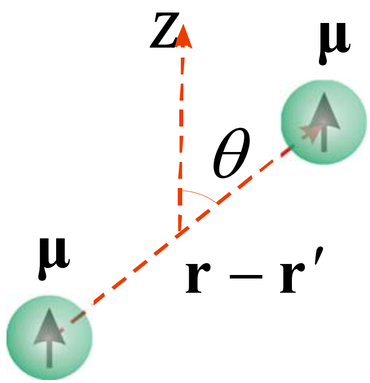
- ☑ Introduction: dipole-dipole interaction (DDI)
- ☑ Dipolar spin-1 condensate
  - ➢ Weak DDI
  - ➢ Strong DDI
- ☑ Polarized dipolar lattice models
  - ➢ 2D isotropic model in square lattice
  - ➢ 2D anisotropic model in square lattice
  - ➢ 3D cubic lattice
- ☑ Summary and outlook

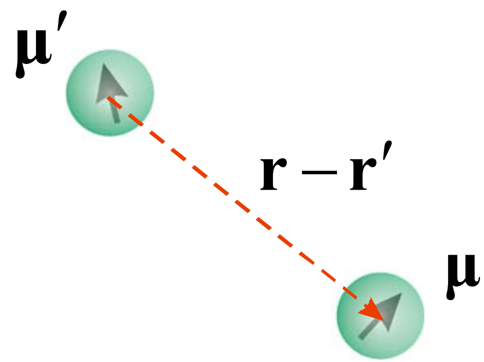
Interactions between ultra-cold atoms

☑ Short-range interaction

$$V_0(\mathbf{r},\mathbf{r}') = \frac{4\pi\hbar^2 a_{\mathrm{sc}}}{m}\,\delta(\mathbf{r}-\mathbf{r}')$$

☑ Dipolar interaction





$$V_{\text{polarized-dipole}} = c_d \frac{1-3\cos^2\theta}{|\mathbf{r}-\mathbf{r}'|^3}$$

$$V_{\text{dipole}} = c_d \frac{\boldsymbol{\mu}\cdot\boldsymbol{\mu}' - 3(\boldsymbol{\mu}\cdot\hat{\mathbf{e}})(\boldsymbol{\mu}'\cdot\hat{\mathbf{e}})}{|\mathbf{r}-\mathbf{r}'|^3}$$

Physics of ultra-cold dipolar bosons

- ☑ Scalar condensate (polarized dipoles)
  - ➢ Ground state (Yi&You, Goral, Santos, Bohn, etc)
  - ➢ Excitation (Yi&You, Santos, O'Dell, Bohn, etc)
  - ➢ Dynamics (Yi&You, Goral, Santos, etc)
  - ➢ Vortex state (Cooper, Zhai, Yi, O'Dell, etc)
  - ➢ Soliton (Santos)
- ☑ Spinor condensate (free dipoles)
  - ➢ Ground state (Yi, Pu, You, Ueda, Machida)
  - ➢ Dynamics (Santos, Ueda, Lewenstein)
- ☑ Optical lattice
  - ➢ Lattice spin models (Pu, Zoller, Demler, etc)
  - ➢ Polarized dipoles (Goral, Santos, Lewenstein, Yi, Wang, etc)
  - ➢ Two-body system (You)
- ☑ Other problems: finite temperature, Wigner crystal, etc

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How strong is dipolar interaction?

☑ Magnetic dipole moment:

$$c_d / g \approx 0.1\mu^2 / a_{sc} \ll 1$$

In general, it's difficult to observe the dipolar effects in atomic system, BUT…

$^{52}\mathrm{Cr}\ (\mu = 6)$ *Griesmaier, et al., PRL* ***94****, 160401 (2005).*

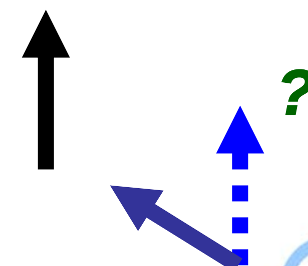
☑ Electric dipole moment:

$$c_d / g = 2.3 \times 10^3 d^2 / a_{sc}$$

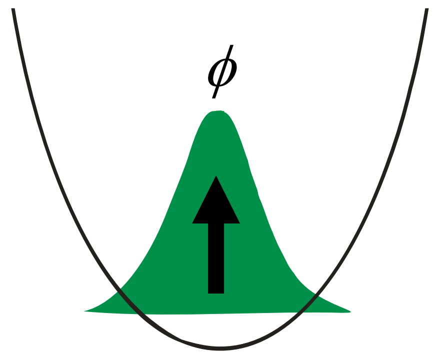
☑ Spinor condensate with magnetic dipolar interaction

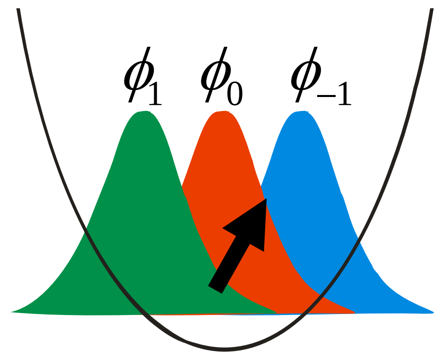
Dipolar effects may be amplified if dipoles are free.

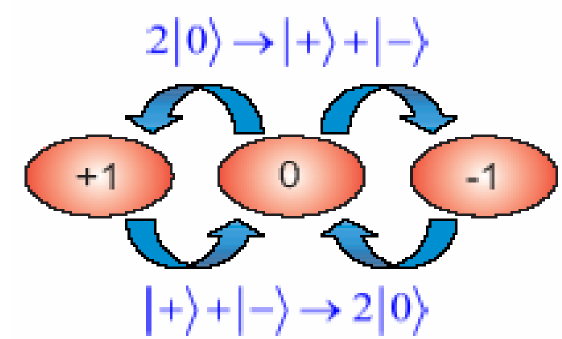
Free dipole ➔➔ multiple-component BEC.



Spin-1 condensate







$$V_{\text{collision}}(\mathbf{r}_1, \mathbf{r}_2) = (c_0 + c_2 \mathbf{F}_1 \cdot \mathbf{F}_2)\delta(\mathbf{r}_1 - \mathbf{r}_2)$$

$$c_2 \begin{cases} < 0 \;\; \Rightarrow \text{Ferromagnetic} \\ > 0 \;\; \Rightarrow \text{Anti-ferromagnetic} \end{cases} \qquad |c_2| \sim 0.01 c_0$$

*Ho, PRL **81**, 742 (1998).*
*Ohmi et al., J. Phys. Soc. Jpn. **67**, 1822 (1998).*

Dipolar spin-1 condensate

$$\mathcal{H}_{\rm tot} = \underbrace{T + U} + V_{\text{spin-indep}} + V_{\text{exchange}} + V_{\text{dipole}}$$

$$\int d\mathbf{r}\,\psi_\alpha^\dagger(\mathbf{r})\left[-\frac{\hbar^2\nabla^2}{2m} + U(\mathbf{r})\right]\psi_\alpha(\mathbf{r})$$

$$\frac{c_0}{2}\int d\mathbf{r}\,\psi_\alpha^\dagger(\mathbf{r})\psi_\beta^\dagger(\mathbf{r})\psi_\alpha(\mathbf{r})\psi_\beta(\mathbf{r})$$

$$\frac{c_2}{2}\int d\mathbf{r}\,\psi_\alpha^\dagger(\mathbf{r})\psi_\delta^\dagger(\mathbf{r})\mathbf{F}_{\alpha\beta}\cdot\mathbf{F}_{\delta\gamma}\psi_\beta(\mathbf{r})\psi_\gamma(\mathbf{r})$$

$$\frac{c_2}{2}\int\frac{d\mathbf{r}d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\left[\psi_\alpha^\dagger(\mathbf{r})\psi_\delta^\dagger(\mathbf{r}')\mathbf{F}_{\alpha\beta}\cdot\mathbf{F}_{\delta\gamma}\psi_\beta(\mathbf{r})\psi_\gamma(\mathbf{r}') - 3\psi_\alpha^\dagger(\mathbf{r})\psi_\delta^\dagger(\mathbf{r}')\mathbf{F}_{\alpha\beta}\cdot\mathbf{e}\,\mathbf{F}_{\delta\gamma}\cdot\mathbf{e}\,\psi_\beta(\mathbf{r})\psi_\gamma(\mathbf{r}')\right]$$

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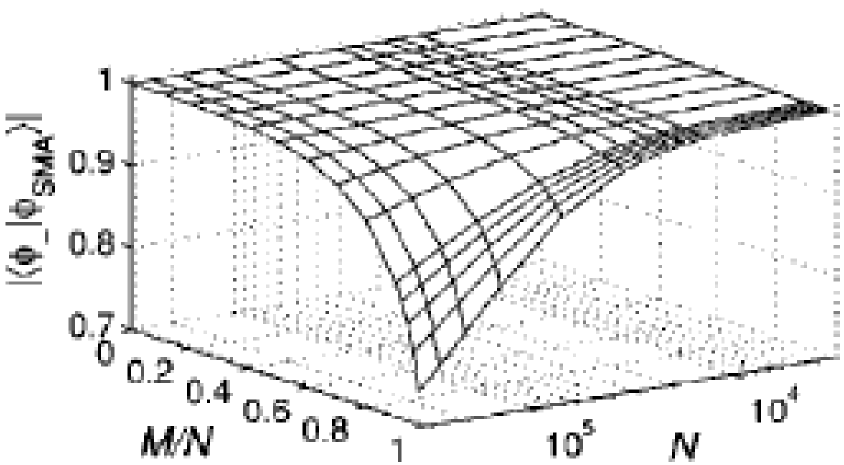
Single-mode approximation (SMA)

All spin components share a common spatial mode function:

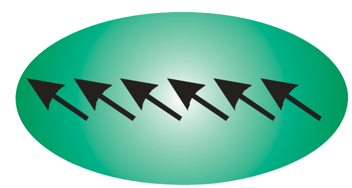
$$\hat{\psi}_\alpha(\mathbf{r}) \simeq \phi(\mathbf{r})\hat{a}_\alpha$$

*Law et al., PRL **81**, 5257 (1998).*



*Yi et al., PRA **66**, 011601 (2002).*

Spins and SMA:



Simplified Hamiltonian

$$\mathcal{H} = (\pm 1 - c)\mathbf{L}^2 + 3c(L_z^2 + n_0)$$

$$\mathbf{L} = a_\alpha^\dagger \mathbf{F}_{\alpha\beta} a_\beta$$

$$a_0^\dagger a_0$$

$$\mathbf{L}^2 |l,m\rangle = l(l+1)|l,m\rangle,$$
$$L_z |l,m\rangle = m|l,m\rangle.$$

$$l = \begin{cases} 0, 2, \cdots, N, & \text{for even } N \\ 1, 3, \cdots, N, & \text{for odd } N \end{cases}$$

$$m = -l, -l+1, \cdots, l$$

$$c \propto V_{\text{dipole}} / V_{\text{exchange}}$$

*Yi, You, and Pu, PRL **93**, 040403 (2004).*

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Quantum phases under weak DDI

$$\mathcal{H} = (\pm 1 - c)\mathbf{L}^2 + 3c(L_z^2 + n_0)$$

- ☑ Ferromagnetic

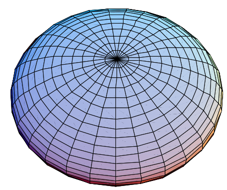
  $|G\rangle_A : |N, 0\rangle$

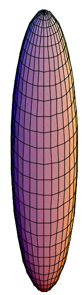
- ☑ Ferromagnetic

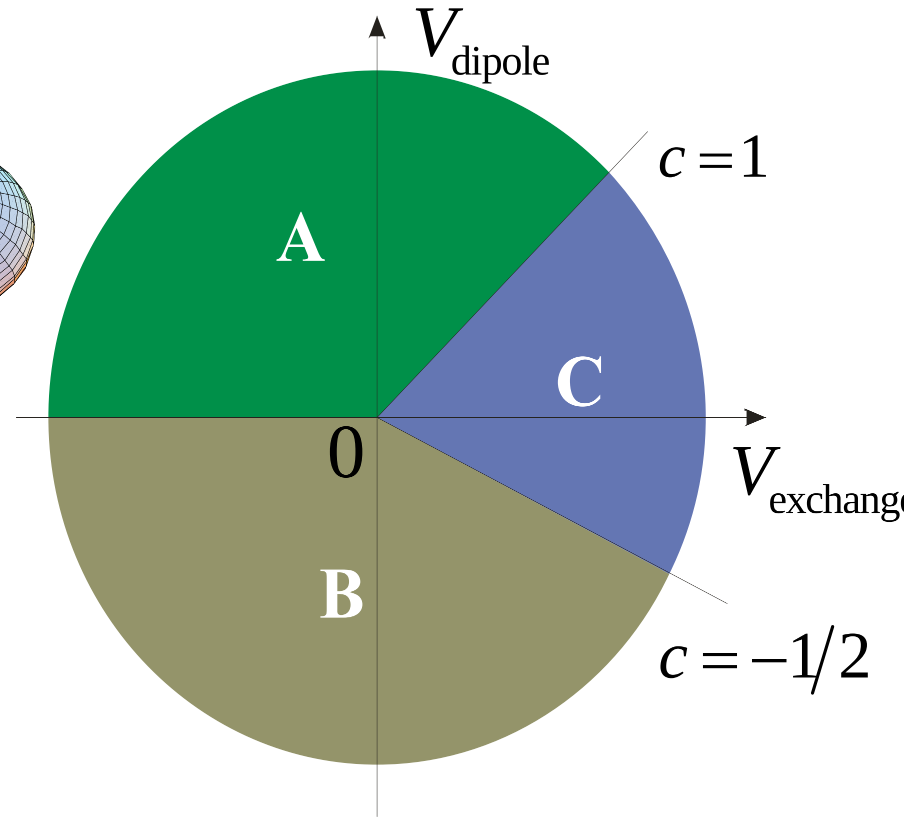
  $|G\rangle_B : |N, \pm N\rangle$

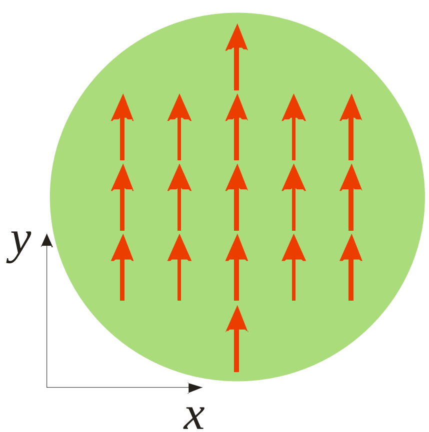
- ☑ Anti-ferromagnetic

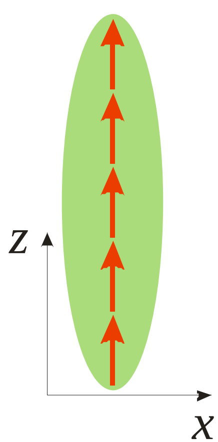
  $|G\rangle_C : |0, 0\rangle$



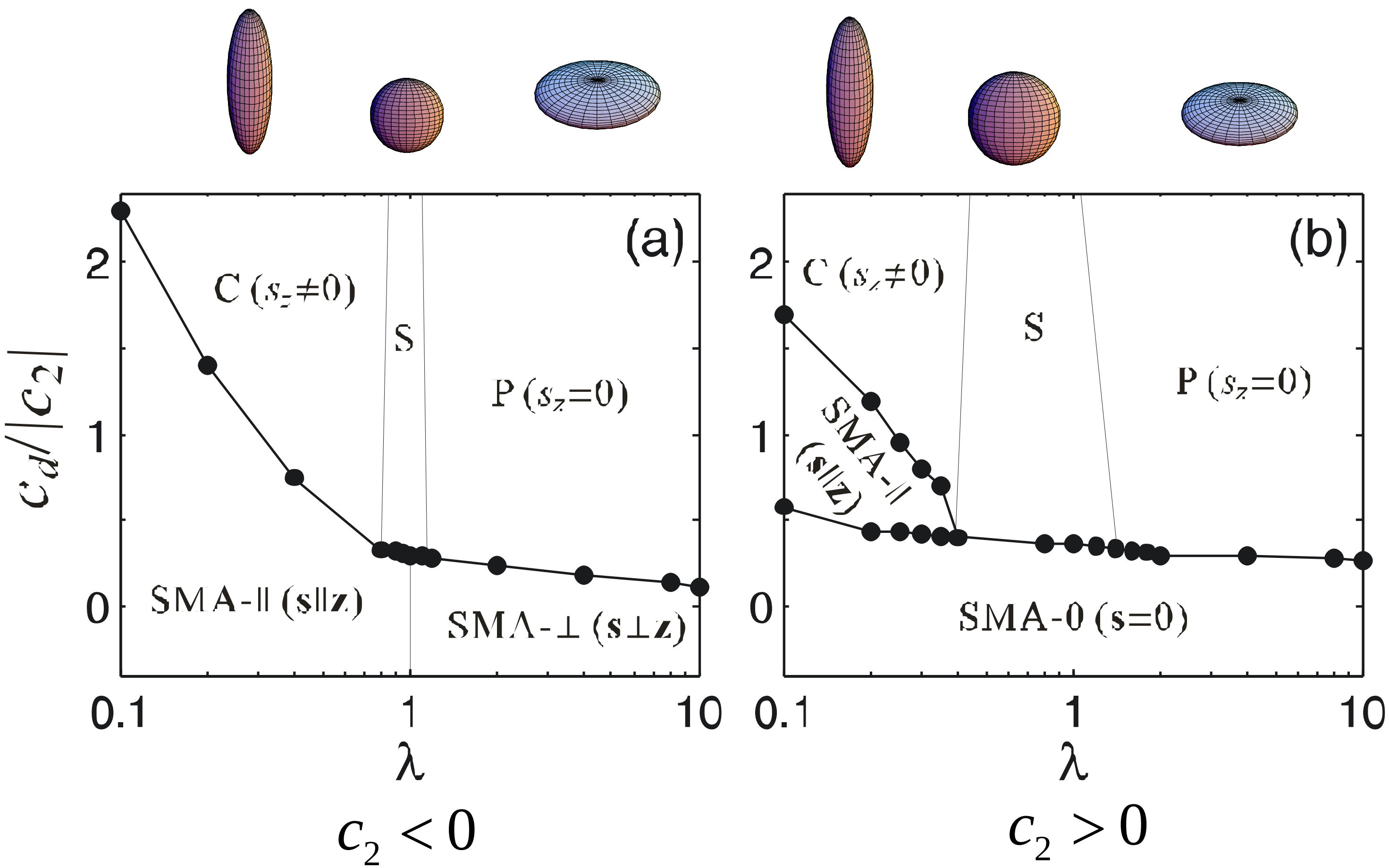








Full mean-field phase diagram



Yi and Pu, PRL **73**, 020401 (2006).

P phase: wave function

☑ Wave functions

$$\phi_\alpha(\mathbf{r}) = \sqrt{n_\alpha(\mathbf{r})}e^{i\Theta_\alpha(\mathbf{r})}$$

☑ Density

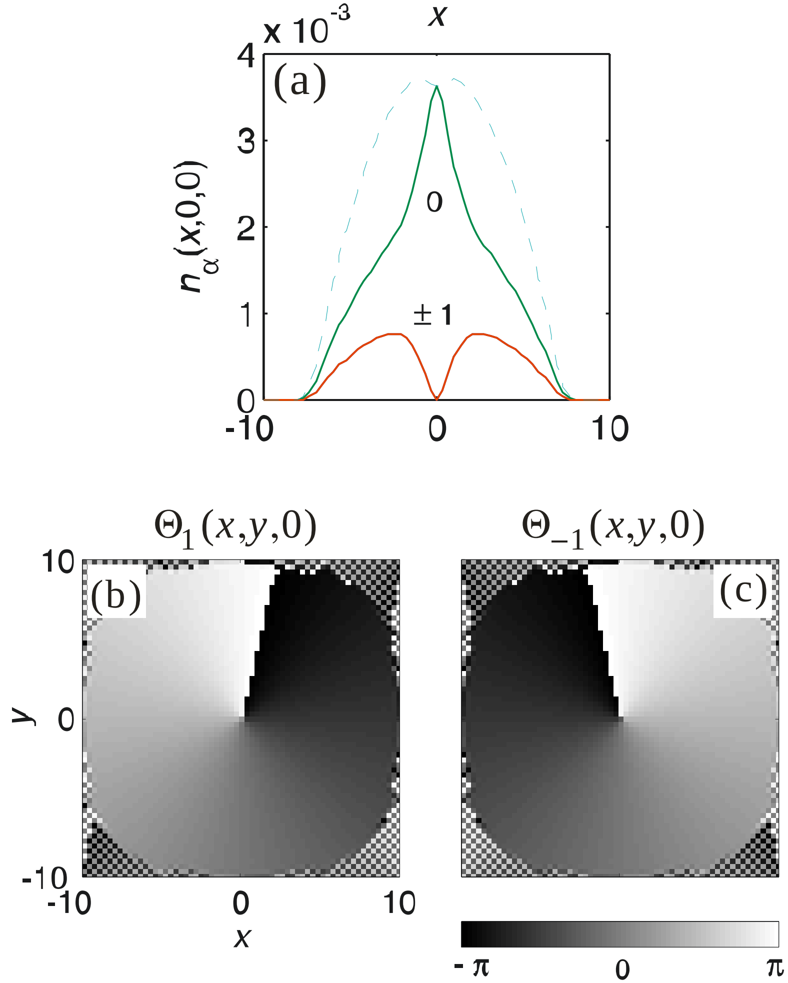
$$n_1(\mathbf{r}) = n_{-1}(\mathbf{r})$$

$n_\alpha(\mathbf{r})$ axially symmetric

☑ Phases

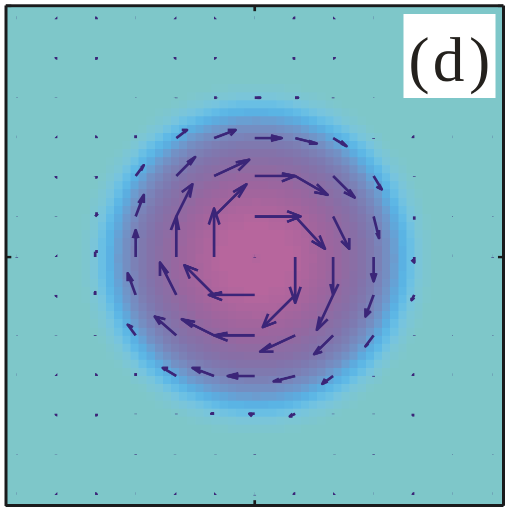
$$\Theta_\alpha = w_\alpha \varphi + \vartheta_\alpha$$

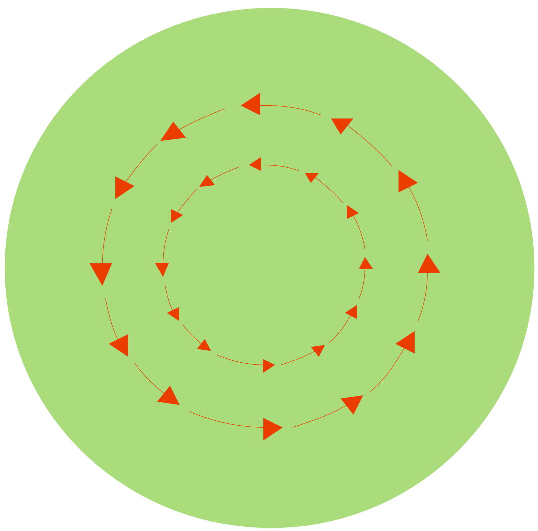
$$(w_1, w_0, w_{-1}) = (-1, 0, 1)$$

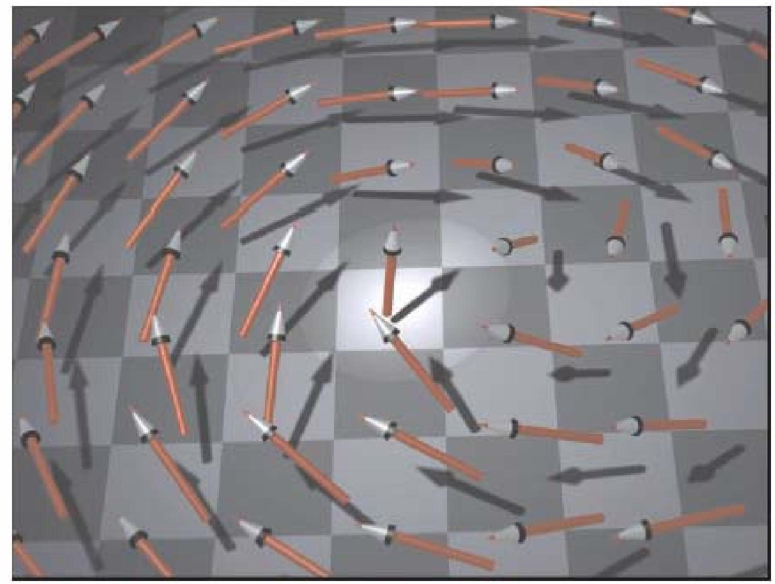


P phase: spin texture

$\mathbf{S}(x,y,0)$







Raabe et al., J. Appl. Phys. ***88****, 4437 (2000).*
Shinjo et al., Science ***289****, 930 (2000).*
Wachoviak et al., Science ***298****, 577 (2002).*

C phase: spin texture

☑ Densities

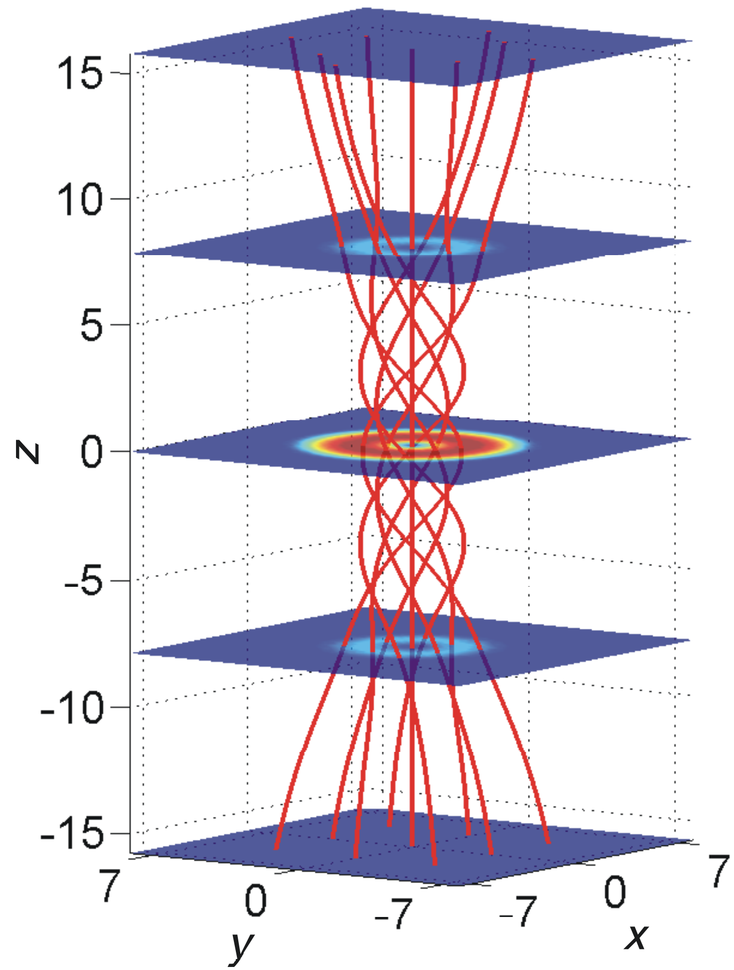
$$n_1(\mathbf{r}) \neq n_0(\mathbf{r}) \neq n_{-1}(\mathbf{r})$$

$$n_\alpha(\mathbf{r}) \text{ axially symmetric}$$

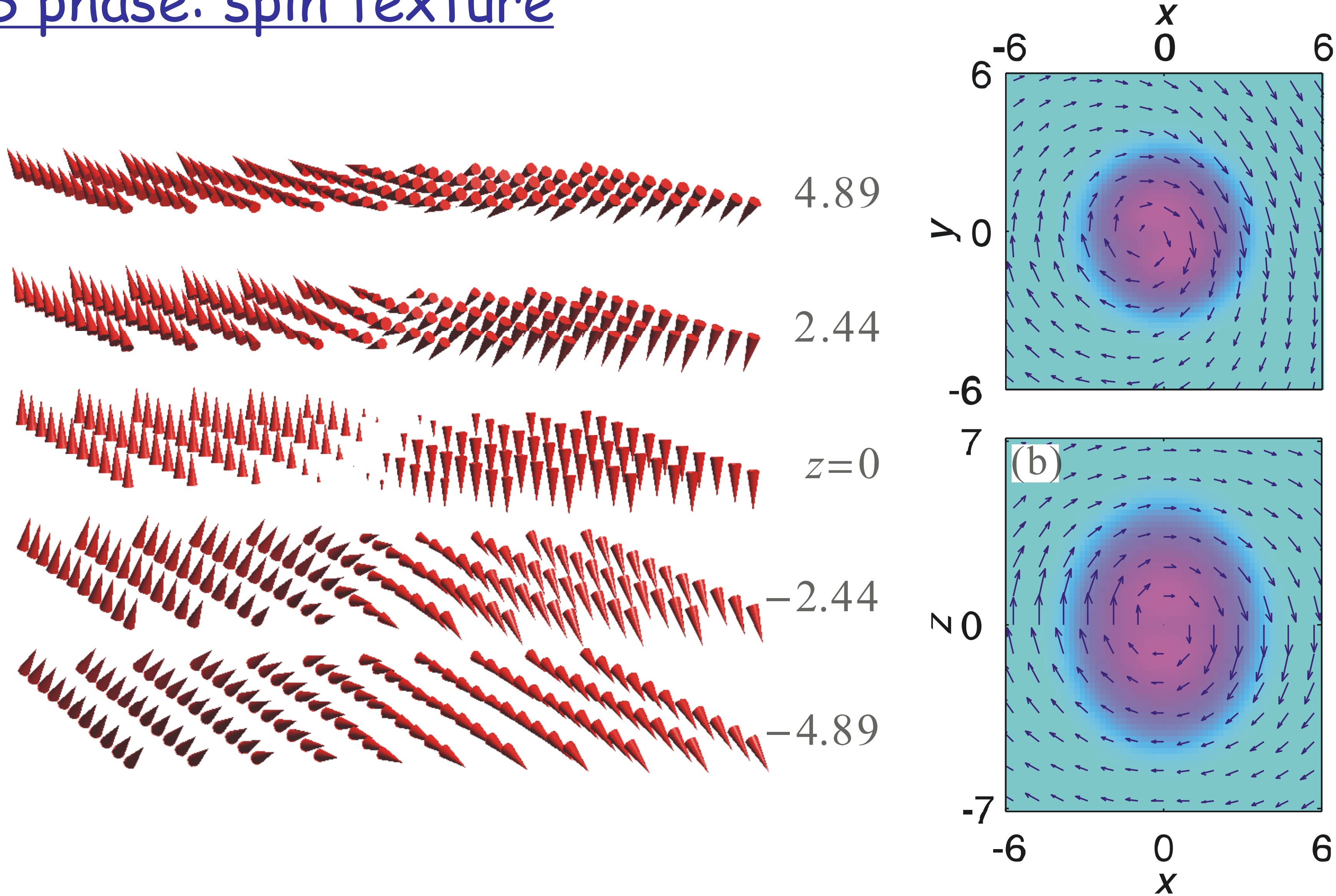
☑ Phases

$$\Theta_\alpha = w_\alpha \varphi + \vartheta_\alpha$$

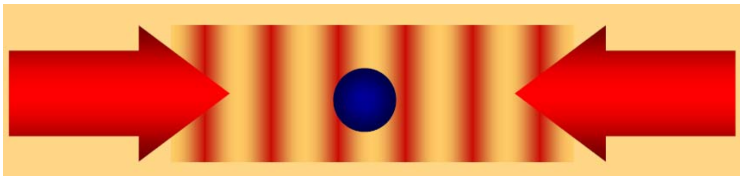
$$\langle w_1, w_0, w_{-1} \rangle = \langle 0, 1, 2 \rangle$$

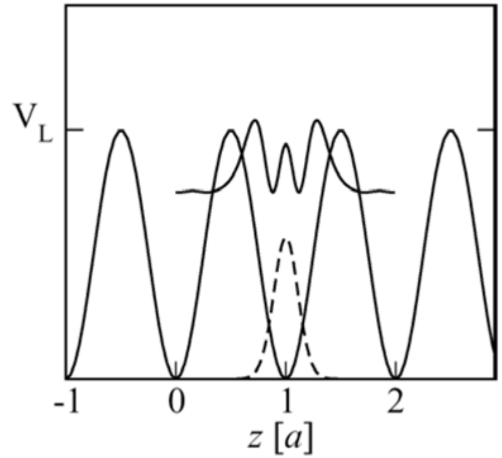


S phase: spin texture



Optical lattices





$\alpha = 2$

$\alpha = 0$

$$V_{ol}(\mathbf{r}) = V_0(\sin^2 kx + \sin^2 ky + \sin^2 kz)$$

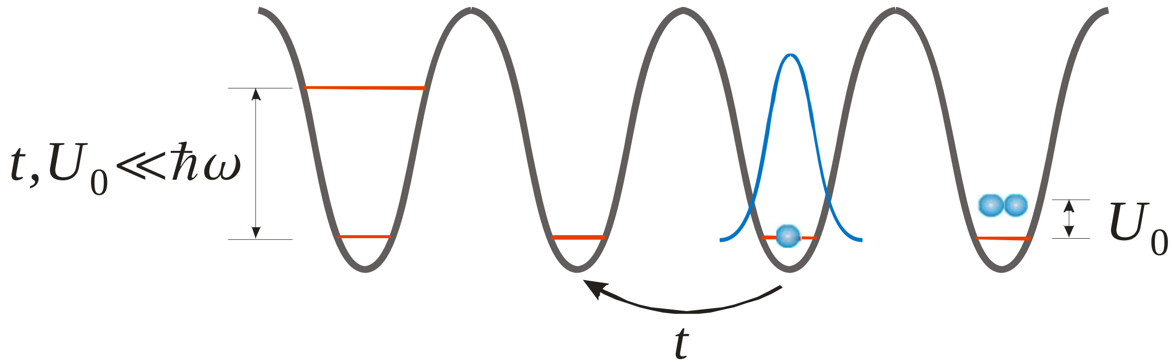
$$k = \frac{\pi}{\lambda}, \quad \lambda = 2a, \quad a \text{ lattice constant}$$

☑ Hamiltonian for the system

$$H = \int d\mathbf{r}\Psi^\dagger(\mathbf{r})\left[-\frac{\hbar^2\nabla^2}{2M} + V_{ol}(\mathbf{r}) - \mu\right]\Psi(\mathbf{r}) + \frac{4\pi\hbar^2 a_s}{M}\int d\mathbf{r}\Psi^\dagger(\mathbf{r})\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})\Psi(\mathbf{r})$$

☑ Expand H in Wannier basis $\quad \Psi(\mathbf{r}) = \sum_{i,\alpha} w_{i,\alpha}(\mathbf{r}) b_{i,\alpha}$

Bose-Hubbard model



☑ Wannier function of lowest energy band

$$w_{i,0}(\mathbf{r}) \equiv w(\mathbf{r}-\mathbf{r}_i)$$

☑ Hamiltonian :

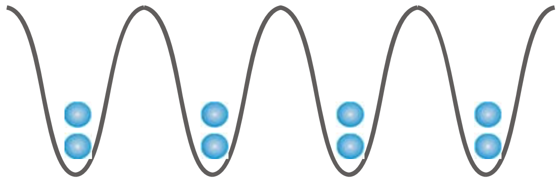
$$H = -t\sum_{\langle i,j\rangle}\left(b_i^\dagger b_j + b_j^\dagger b_i\right) - \mu\sum_i n_i + \frac{U_0}{2}\sum_i n_i\left(n_i - 1\right)$$

➤ $t = \int d\mathbf{r} w_i^*(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2M} + V_{\mathrm{ol}}(\mathbf{r})\right)w_j(\mathbf{r})$

➤ $U_0 = \frac{4\pi\hbar^2 a_s}{M}\int d\mathbf{r}\left|w_i(\mathbf{r})\right|^4$

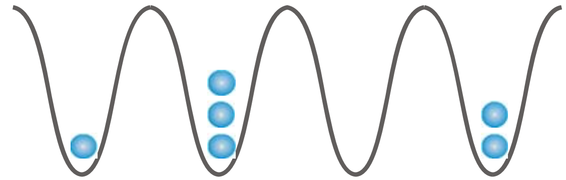
*Jaksch et al., PRL **81**, 3108 (1998)*

Superfluid-Mott insulator transition



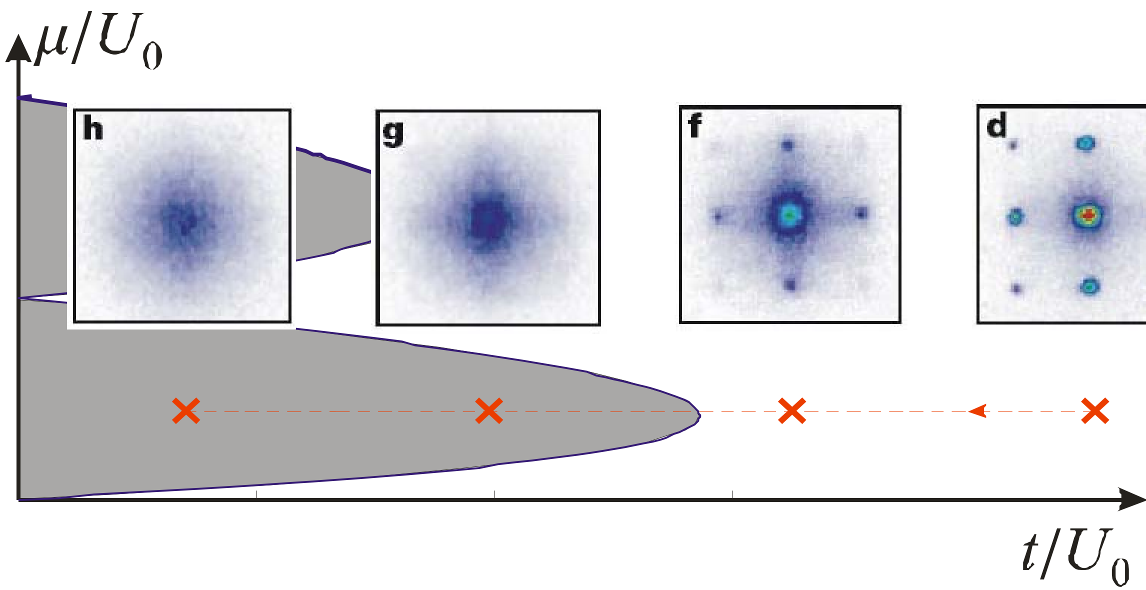
$t/U_0 \ll 1,$ Mott insulator

$\langle b \rangle = 0 \ \& \ \langle n \rangle = 1, 2, \cdots$



$t/U_0 \gg 1,$ Superfluid

$\langle b \rangle \neq 0$



Greiner et al., Nature ***415***, *39 (2002)*

Extended Bose-Hubbard model and supersolid

$$H = -t\sum_{\langle i,j\rangle}\left(b_i^\dagger b_j + b_j^\dagger b_i\right) - \mu\sum_i n_i + \frac{U_0}{2}\sum_i n_i\left(n_i - 1\right)$$

$$+U_1\sum_{\langle i,j\rangle} n_i n_j + U_2\sum_{\langle\langle i,j\rangle\rangle} n_i n_j + \ldots$$

☑ Excited energy band

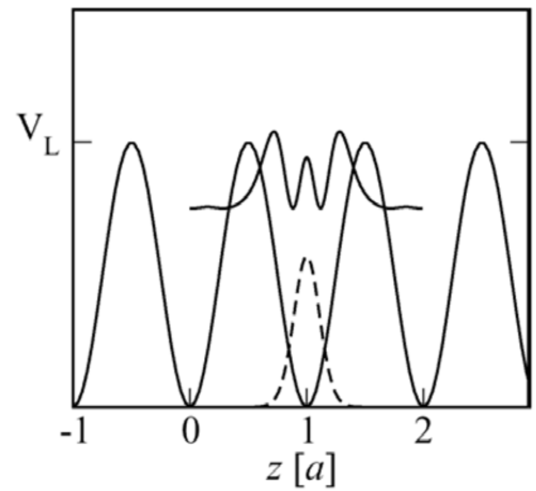
Scarola and Das Sarma, PRL ***95****, 033003 (2005)*

☑ Fermions mediated interaction

Buchler and Blatter, PRL ***91****, 130404 (2003)*

☑ Dipole-dipole interaction

Goral et al., PRL ***88****, 170406 (2002)*

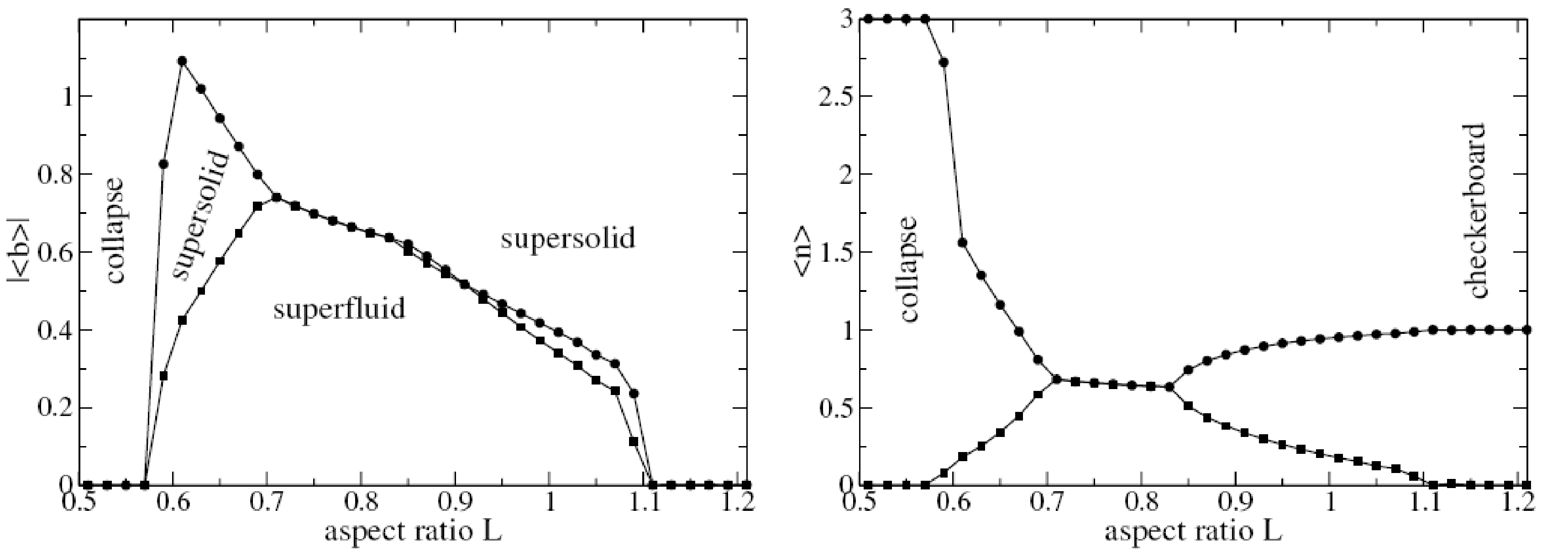


$\alpha = 2$

$\alpha = 0$

Supersolid phase

$$\langle b_i \rangle = 0 \ \& \ \langle n_i \rangle \text{ is periodically modulated}$$

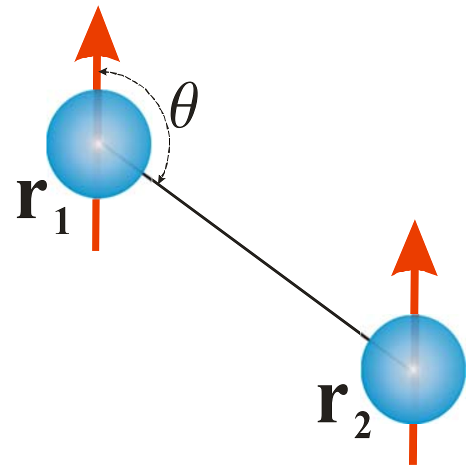


*Goral et al., PRL **88**, 170406 (2002)*

New observation on DDI

☑ DDI between polarized dipoles

$$V_{\mathrm{dd}}(\mathbf{r}_1-\mathbf{r}_2)=c_d\frac{1-3\cos^2\theta}{|\mathbf{r}_1-\mathbf{r}_2|^3}$$

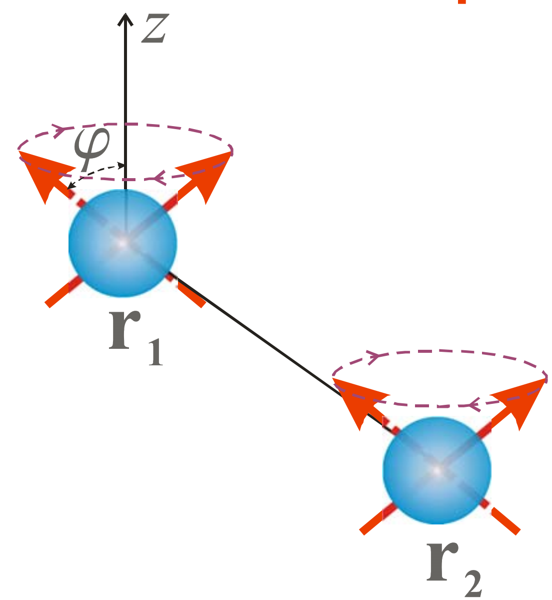


☑ Tuning DDI via a rotating orienting field

$$\langle V_{\mathrm{dd}}(\mathbf{r}_1-\mathbf{r}_2)\rangle=\left(\frac{3\cos^2\varphi-1}{2}\right)c_d\frac{1-3\cos^2\theta}{|\mathbf{r}_1-\mathbf{r}_2|^3}$$

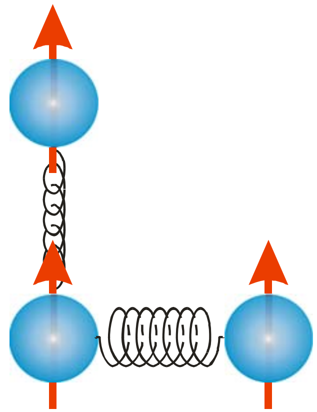
$$\|$$

$$-\frac{1}{2}\le f\le 1$$

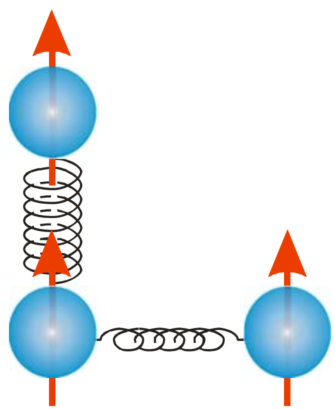


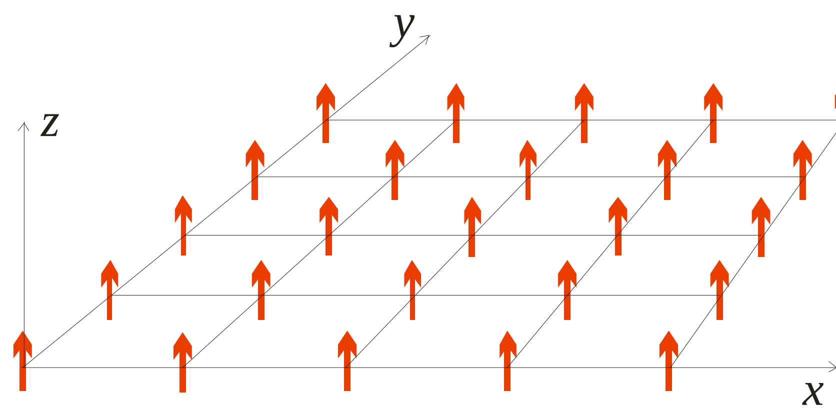
Anisotropic nature of DDI

- ☑ Positive f



- ☑ Negative f





Our Hamiltonian

$$H = -t\sum_{\langle i,j\rangle}\left(b_i^{\dagger}b_j + b_j^{\dagger}b_i\right) - \mu\sum_i n_i + \frac{U_0}{2}\sum_i n_i\left(n_i - 1\right)$$

$$+\frac{1}{2}\cancel{\sum_i U_{\mathrm{dd}}^{ii} n_i\left(n_i - 1\right)} + \frac{1}{2}\sum_{\langle i,j\rangle} U_{\mathrm{dd}}^{ij} n_i n_j$$

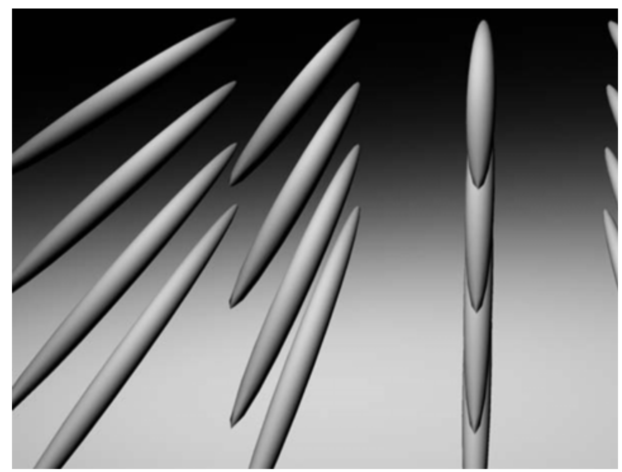
$$w_i(\mathbf{r}) \propto e^{-(\mathbf{r}-\mathbf{r}_i)^2/(2\sigma^2)}$$

☑ DDI: $U_{\mathrm{dd}}^{ij} = f c_d \mathcal{D}_{ij}$

$$= f c_d \int d\mathbf{r}d\mathbf{r}'\left|w_i(\mathbf{r})\right|^2 \frac{1-3\cos^2\theta}{\left|\mathbf{r}-\mathbf{r}'\right|^3}\left|w_j(\mathbf{r}')\right|^2$$

$$\sigma = \frac{a}{\pi}\left(\frac{V_0}{\hbar^2 k^2/2M}\right)^{-1/4}$$

- $U_{\mathrm{dd}}^{ii} = 0$
- $\mathcal{D}_{ij} \equiv \mathcal{D}_{(l_x l_y l_z)} : \mathbf{r}_i - \mathbf{r}_j = a\left(l_x\hat{\mathbf{x}} + l_y\hat{\mathbf{y}} + l_z\hat{\mathbf{z}}\right)$
- $-l_{\mathrm{cutoff}} \le l_x, l_y, l_z \le l_{\mathrm{cutoff}}$
- $\gamma = \dfrac{f c_d}{4\pi\hbar^2 a_s / M}$



*Yi, Li, and Sun, PRL **98**, 260405 (2007).*

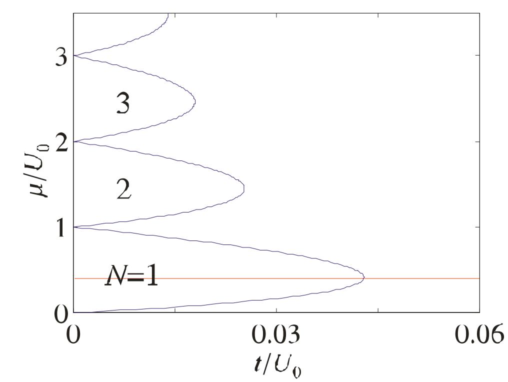
Gutzwiller variational wave function

$$|\Psi\rangle = \prod_{i=1}^{N_s} |\psi\rangle_i$$

$$||$$

$$|\psi\rangle_i = \sum_{n=0}^{\infty} f_n^{(i)} |n\rangle_i, \qquad \sum_{n=0}^{\infty} \left| f_n^{(i)} \right|^2 = 1$$

- ☑ $f_n^{(i)}$ is obtained by minimizing $E = \langle \Psi | H | \Psi \rangle$
- ☑ Fixed Chemical potential $\mu = 0.4U_0$
- ☑ Periodic boundary condition
- ☑ Identifying quantum phases



- ➢ Superfluid order

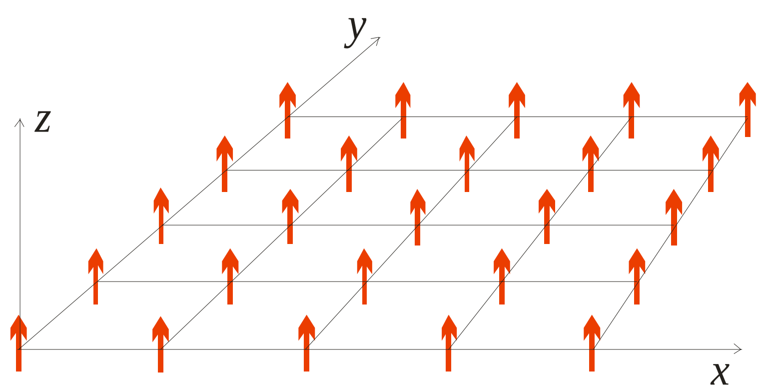
  $|\langle b_i \rangle| \neq 0$

- ➢ Density wave order

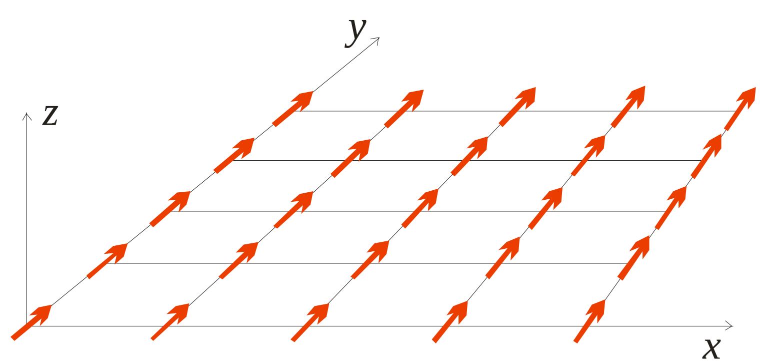
  $\langle n_i \rangle$ is periodically modulated

3 models to be studied

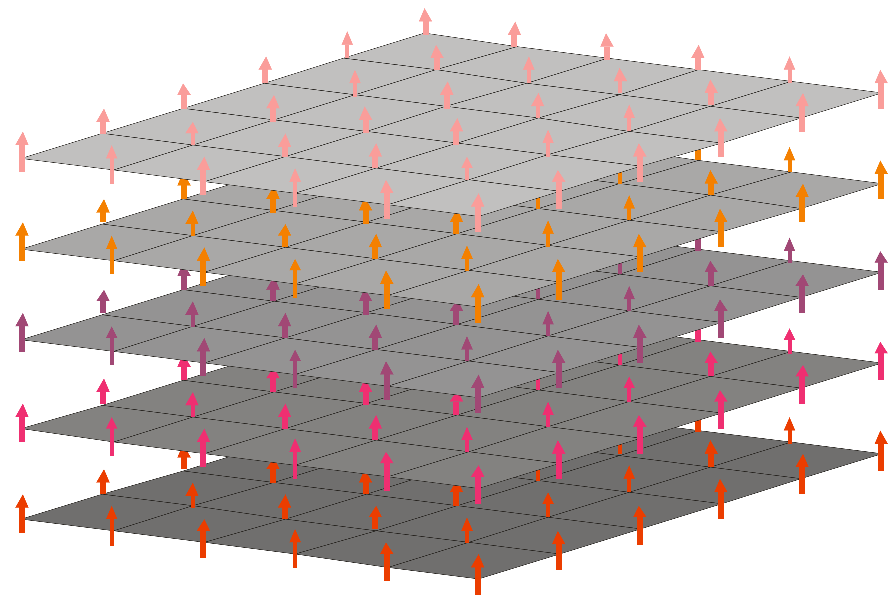
☑ 2D isotropic model



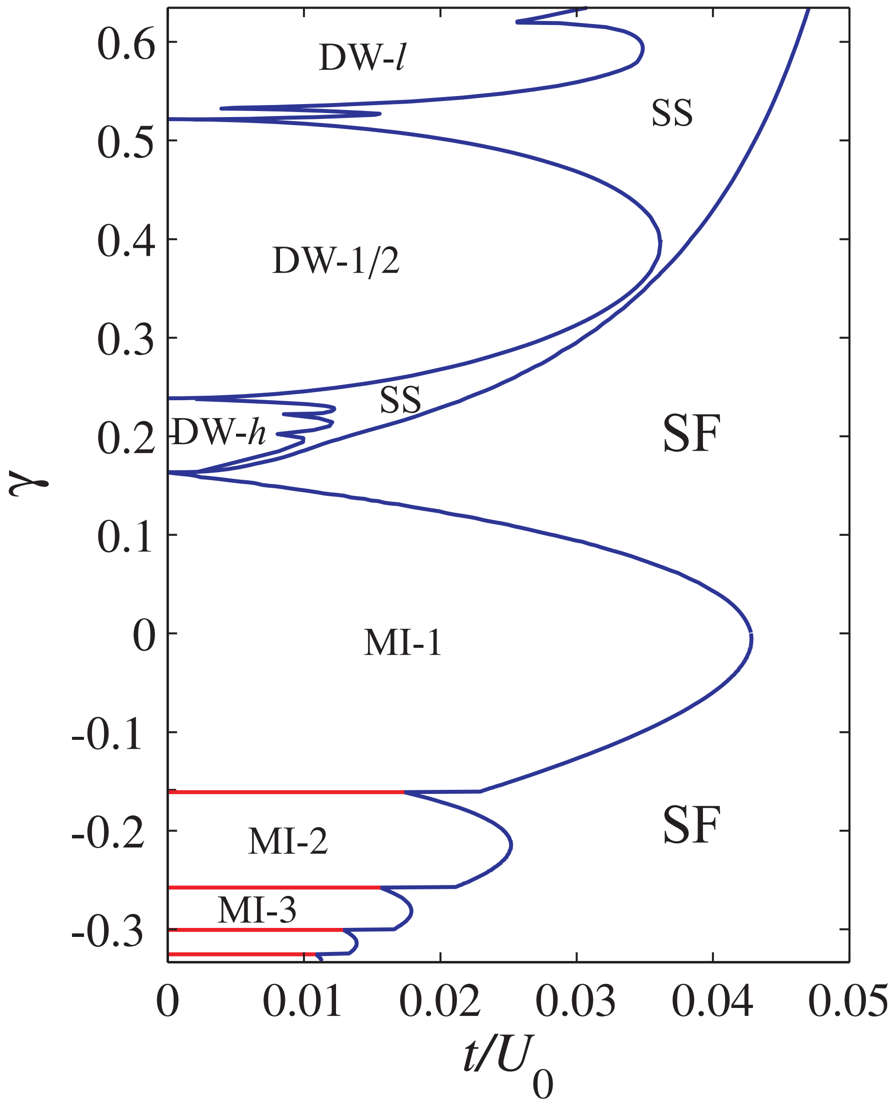
☑ 2D anisotropic model

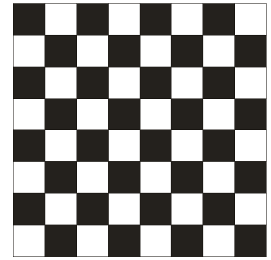


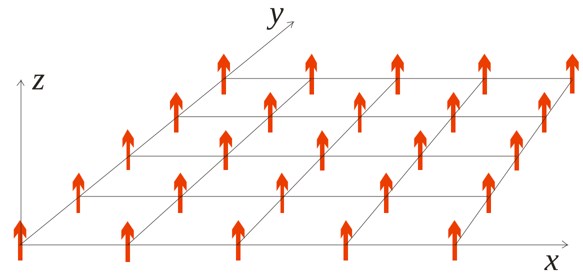
☑ 3D lattice



2D isotropic: phase diagram

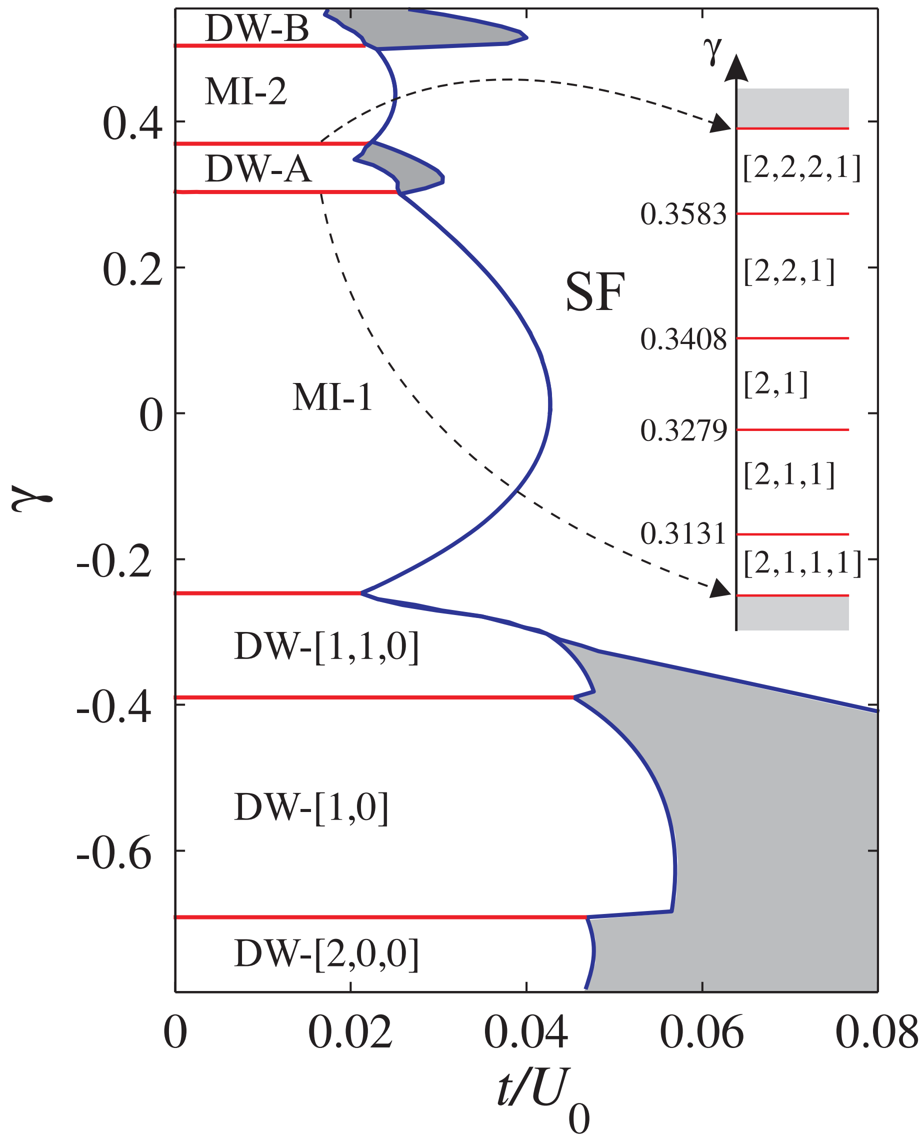


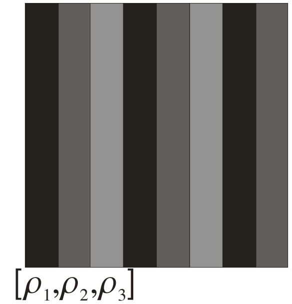


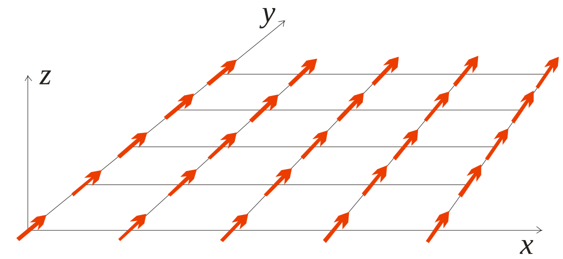


- ☑ Negative γ
  - ➢ Superfluid phase
  - ➢ Mott insulator phases with various mean densities
  - ➢ Effective chemical potential
  - ➢ Unstable for large $\gamma < -0.41$
- ☑ Positive γ
  - ➢ Superfluid phase
  - ➢ Mott insulator phase with unit density
  - ➢ Density wave phases
  - ➢ Supersolid phase
- ☑ Relation between DDI and translational symmetry

2D anisotropic: phase diagram

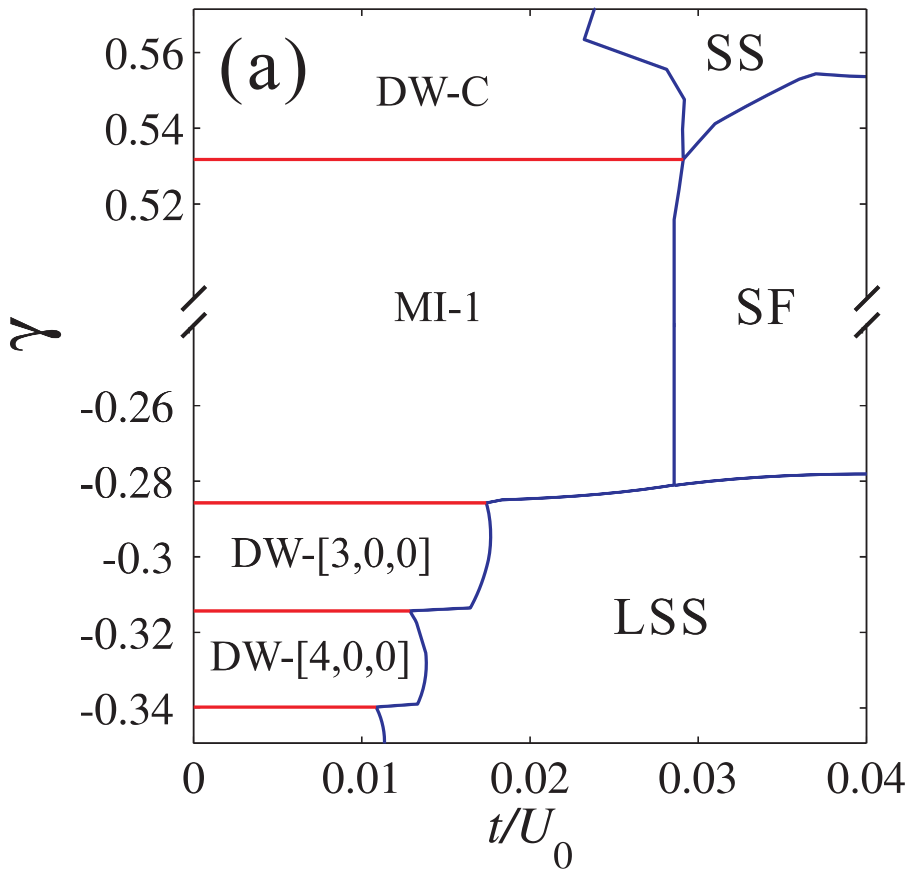


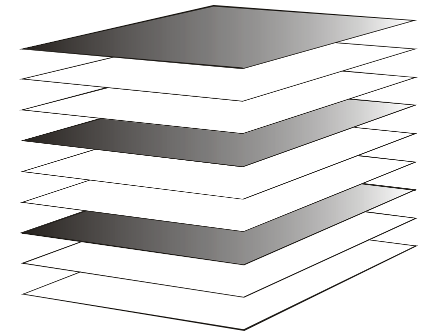




- ☑ MI phases
- ☑ SF phase
- ☑ Striped MI and SF phases
  - ➢ ρ is a constant along attractive direction
  - ➢ ρ is periodically modulated along repulsive direction
  - ➢ Structure is specified as $[\rho_1, \rho_2, \ldots, \rho_m]$
- ☑ Subtle difference between $\gamma \lessgtr 0$
  - ➢ Overall attractive for $\gamma>0$
  - ➢ Overall repulsive for $\gamma<0$
- ☑ Only stable for $-0.63 \leq \gamma \leq 1.27$

3D lattices: phase diagram





☑ Positive γ

- MI and SF phases
- DW-C and SS phases: density modulated periodically on *xy*-plane while constant on *z*-axis
- No checkerboard phase
- Unstable for γ>0.63

☑ Negative γ

- MI and SF phases
- Layered MI and SF phases: one high density layer, and two identical low density layers
- Unstable for γ<-0.41

Conclusions

- ☑ High tunability of DDI
- ☑ Experimental accessibility
  - Chromium atom
  - Polar molecules
  - Rydberg atoms
- ☑ Extremely rich in quantum phases

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Thank you

for your attention

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