Spin-1 Bosons in Optical Lattice

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New Year's Meeting

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  - Mean-field approximation
  - Landau expansion
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- Motivation
  - Spin provides new degrees of freedom
  - Richer quantum phase diagram with different superfluid and insulating phases
  - Model system to study quantum magnetism

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  - Magnetical traps can capture only one hyperfine component

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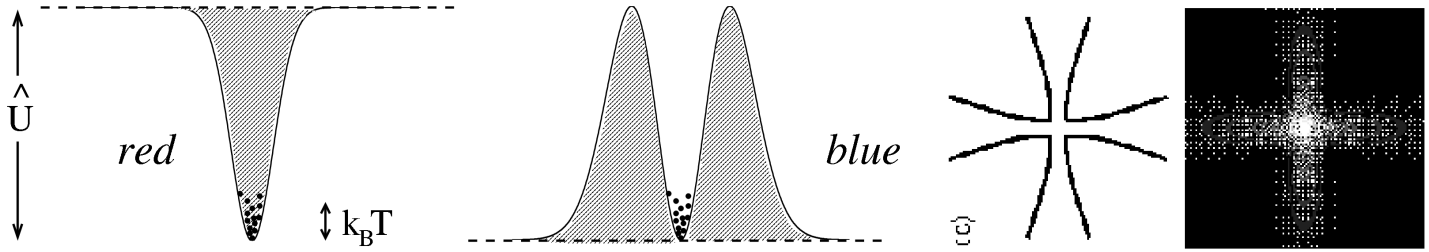
  - Model system to study quantum magnetism
- Obstacles
  - Harmonic trap in addition to lattice needed
  - Magnetical traps can capture only one hyperfine component
- Purely optical traps capture atoms regardless of their hyperfine state

Optical trap

- Far detuned lasers induce electric dipole moments
- Electric forces push atoms towards center of trap (Stark effect)
  - Red detuned light ⇒ Atoms are pushed to maximal intensity
  - Blue detuned light ⇒ Atoms are pushed to minimal intensity
- Very shallow, depth smaller than 1mK



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- Far detuned lasers induce electric dipole moments
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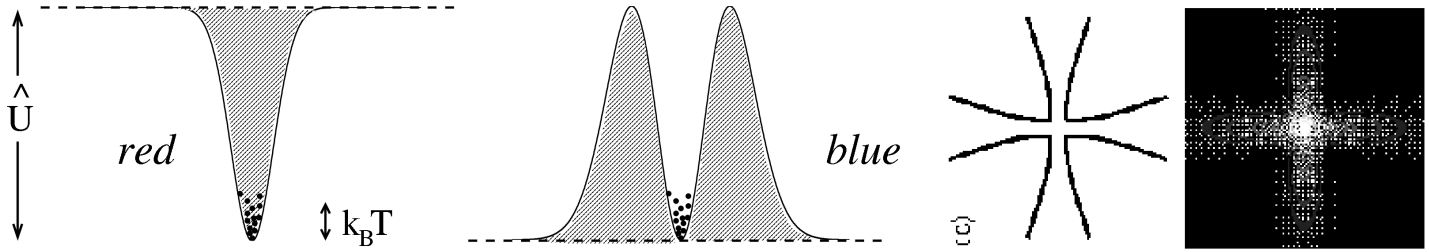
  - Red detuned light ⇒ Atoms are pushed to maximal intensity
  - Blue detuned light ⇒ Atoms are pushed to minimal intensity
- Very shallow, depth smaller than 1mK
- No evaporative cooling possible. Condensate must be produced first in an magnetic trap and then reloaded to an optical one



2nd quantized Hamiltonian for magnetized spin-1 bosons

$$\hat{H} = \sum_{\alpha} \int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x}) \left[-\frac{\hbar^2}{2M}\nabla^2 + V_0 \sum_{j=1}^{D} \sin^2(k_L x_j) - \mu \right] \hat{\Psi}_\alpha(\mathbf{x})$$
$$- \eta \sum_{\alpha,\beta} \int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x}) F^z_{\alpha\beta} \hat{\Psi}_\beta(\mathbf{x})$$
$$+ \frac{c_0}{2} \sum_{\alpha,\beta} \int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x}) \hat{\Psi}^\dagger_\beta(\mathbf{x}) \hat{\Psi}_\beta(\mathbf{x}) \hat{\Psi}_\alpha(\mathbf{x})$$
$$+ \frac{c_2}{2} \sum_{\alpha,\beta,\gamma,\delta} \int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x}) \hat{\Psi}^\dagger_\gamma(\mathbf{x}) \mathbf{F}_{\alpha\beta} \mathbf{F}_{\gamma\delta} \hat{\Psi}_\delta(\mathbf{x}) \hat{\Psi}_\beta(\mathbf{x})$$

Hopping not spin-dependent
Only s-wave scattering, described by pseudopotential

Experimental parameters

$c_0 = 4\pi\hbar^2(a_0 + 2a_2)/3M$: spin independent interaction

$c_2 = 4\pi\hbar^2(a_0 - a_2)/3M$: spin dependent interaction

a_F: s-wave scattering length for total hyperfine spin F

η: magnetic chemical potential to keep magnetization fixed

	$c_2 < 0$ ferromagnetic example ^{87}Rb	$c_2 > 0$ antiferromagnetic example ^{23}Na
a_0	$50\,a_B$	$101.8\,a_B$
a_2	$55\,a_B$	$100.4\,a_B$

$T = 0$, $J = 0$ and $\eta = 0$: anti-ferromagnets try to form singlet pairs on every site
Disturbed by finite temperature, hopping or magnetization

Bose-Hubbard Hamiltonian

Wannier decomposition yields Bose-Hubbard model:

$$\hat{H}_{\mathrm{BH}} = \hat{H}^{(0)} + \hat{H}^{(1)}$$

$$\hat{H}^{(0)} = \sum_i \left[\frac{1}{2} U_0 \hat{n}_i (\hat{n}_i - 1) + \frac{1}{2} U_2 (\hat{\mathbf{S}}_i^2 - 2\hat{n}_i) - \mu \hat{n}_i - \eta \hat{S}_i^z \right]$$

$$\hat{H}^{(1)} = -J \sum_\alpha \sum_{<i,j>} \hat{a}_{i\alpha}^\dagger \hat{a}_{j\alpha}$$

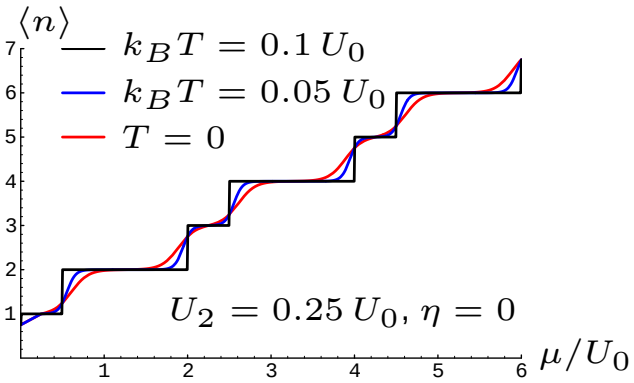
J: tunnel matrix element between nearest neighbors
$U_{0,2} \propto c_{0,2}$: spin independent and dependent interaction
$\hat{n}_i$: particle number operator on site i
$\hat{\mathbf{S}}_i$: spin operators on site i with $[\hat{S}_j^\alpha, \hat{S}_k^\beta] = i\delta_{jk} \sum_\gamma \epsilon_{\alpha\beta\gamma} \hat{S}_j^\gamma$

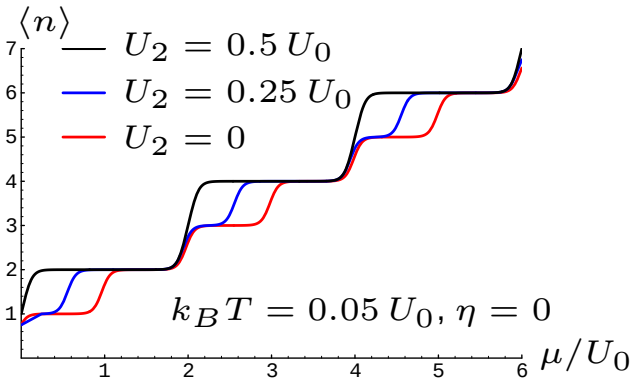
Thermal properties of $J = 0$ system

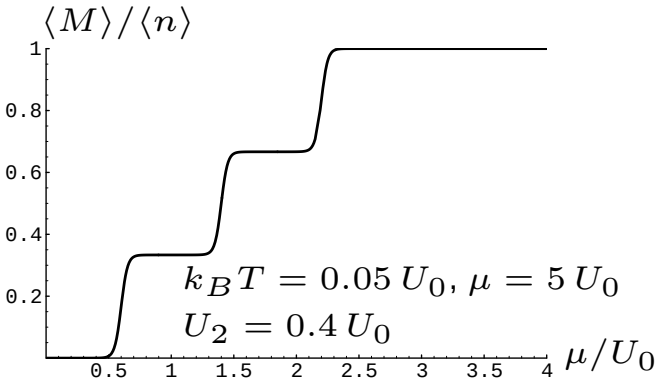
Hamiltonian site diagonal. Eigenstates characterized by particle number n, total spin S and z-component of spin m.

$$\hat{H}^{(0)}|S,m,n\rangle = N_S E^{(0)}_{S,m,n}|S,m,n\rangle$$

$$E^{(0)}_{S,m,n} = \frac{1}{2}U_0 n(n-1) + \frac{1}{2}U_2[S(S+1) - 2n] - \mu n - \eta m$$







Mean-field approximation

- Decoupling the hopping term

$$\hat{a}^\dagger_{i\alpha}\hat{a}_{j\alpha} \approx \Psi_\alpha \hat{a}^\dagger_{i\alpha} + \Psi^*_\alpha \hat{a}_{j\alpha} - \Psi^*_\alpha \Psi_\alpha \,, \quad \Psi_\alpha = \langle \hat{a}_{i\alpha} \rangle \,, \quad \Psi^*_\alpha = \langle \hat{a}^\dagger_{i\alpha} \rangle$$

$$\hat{H}^{(1)}_{\mathrm{MF}} = -Jz \sum_i \sum_\alpha \left(\Psi_\alpha \hat{a}^\dagger_{i\alpha} + \Psi^*_\alpha \hat{a}_{i\alpha} - \Psi^*_\alpha \Psi_\alpha \right) \qquad z = 2D$$

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- Perturbative expansion in $\hat{H}^{(1)}_{\mathrm{MF}}$ needs:

$$\begin{aligned} \hat{a}^\dagger_\alpha |S,m,n\rangle =& M_{\alpha,S,m,n} |S{+}1, m{+}\alpha, n{+}1\rangle \\ &+ N_{\alpha,S,m,n} |S{-}1, m{+}\alpha, n{+}1\rangle \\ \hat{a}_\alpha |S,m,n\rangle =& O_{\alpha,S,m,n} |S{+}1, m{-}\alpha, n{-}1\rangle \\ &+ P_{\alpha,S,m,n} |S{-}1, m{-}\alpha, n{-}1\rangle \end{aligned}$$

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- Matrix elements M, N, O, P calculated by recursion relation

Landau Expansion

- Expanding the grand-canonical free energy

$$\begin{aligned}\mathcal{F}(\mathbf{\Psi}^*, \mathbf{\Psi}) &= -\, k_B T \log \mathrm{Tr}\left\{ e^{-(\hat{H}^{(0)} + \hat{H}^{(1)}_{\mathrm{MF}})/k_B T} \right\} \\ &= -\, k_B T \log \mathcal{Z}^{(0)} + \sum_{\alpha} A^{(2)}_{\alpha} |\Psi_\alpha|^2 + O(\mathbf{\Psi}^4)\end{aligned}$$

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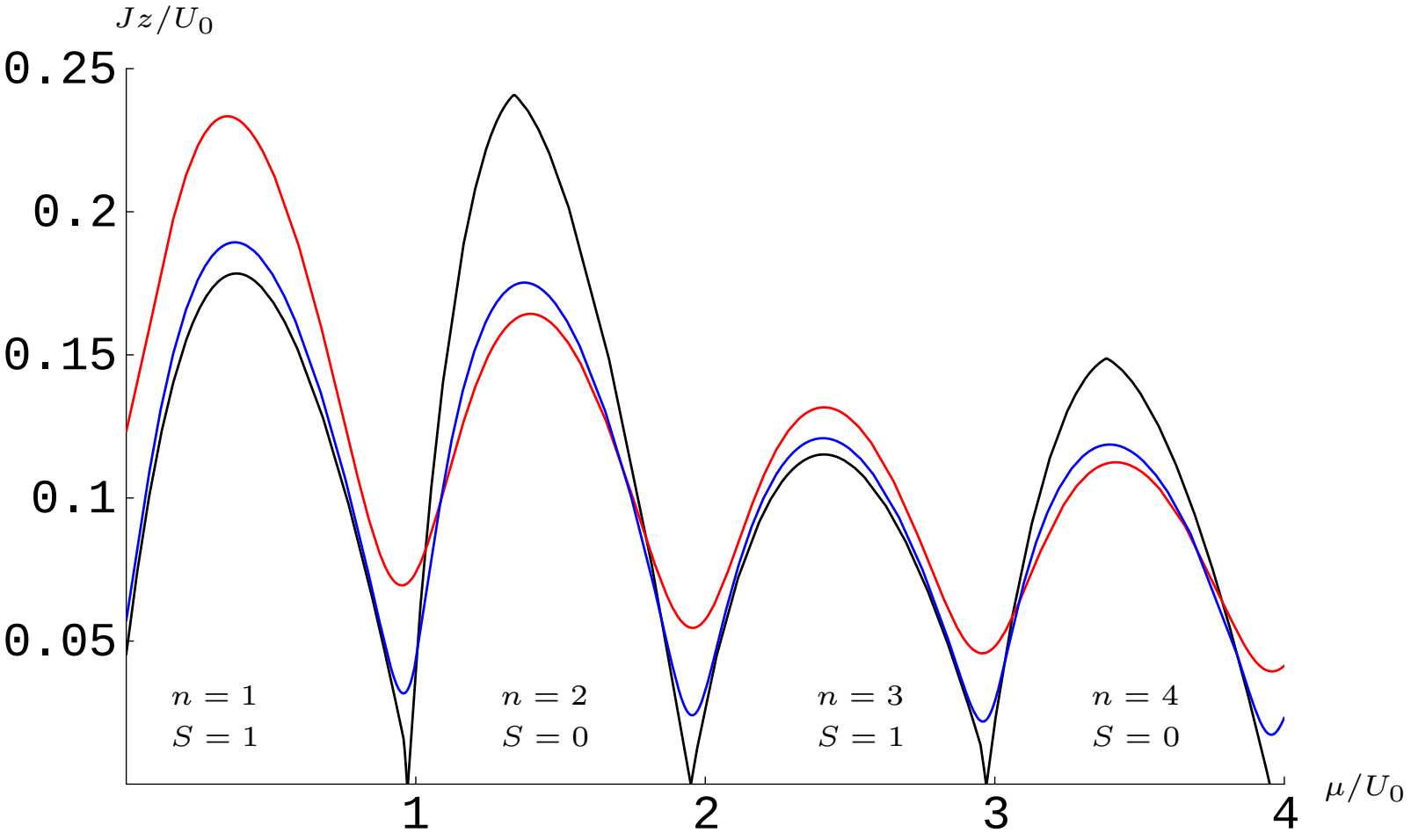
$$= -\, k_B T \log \mathcal{Z}^{(0)} + \sum_{\alpha} A^{(2)}_{\alpha} |\Psi_\alpha|^2 + O(\mathbf{\Psi}^4)$$

- Phase transition occurs when one of the coefficients $A^{(2)}_{\alpha}$ vanishes: different superfluid phases exist
  Magnetized gas ($\eta \neq 0$): $\Psi_1 \neq 0$ or $\Psi_{-1} \neq 0$
  Unmagnetized gas ($\eta = 0$): $\Psi_0 \neq 0$

Quantum phase diagram for different temperatures



$U_2 = 0.04\,U_0$, $\eta = 0.05\,U_0$,
$k_BT = 0.05\,U_0$ (red), $k_BT = 0.02\,U_0$ (blue), $k_BT = 0$ (black)

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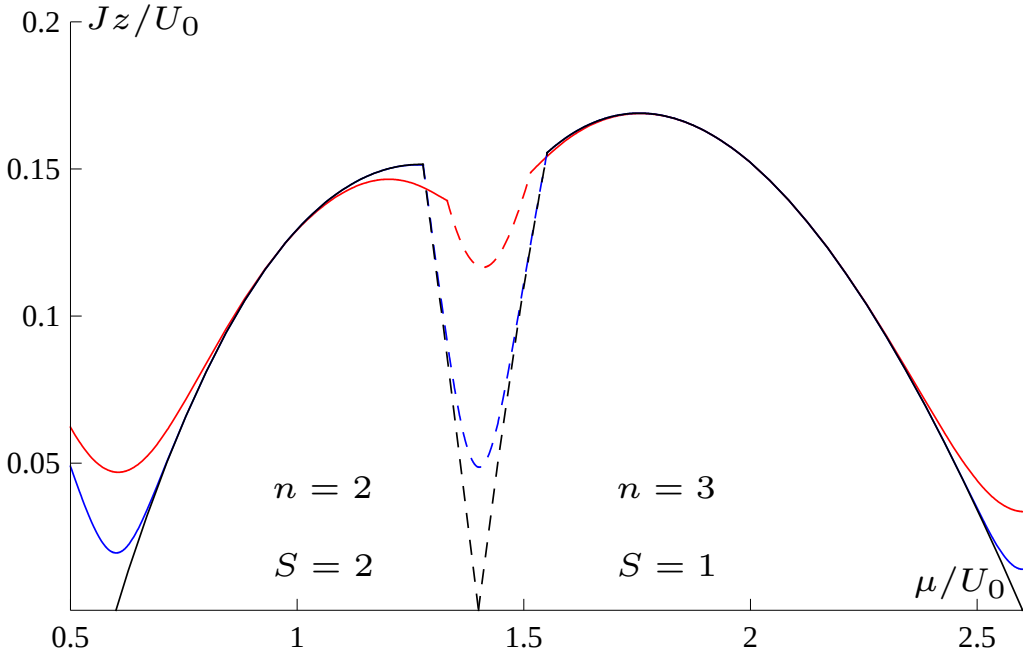

Solid: $\Psi_1 \neq 0$, Dashed: $\Psi_{-1} \neq 0$
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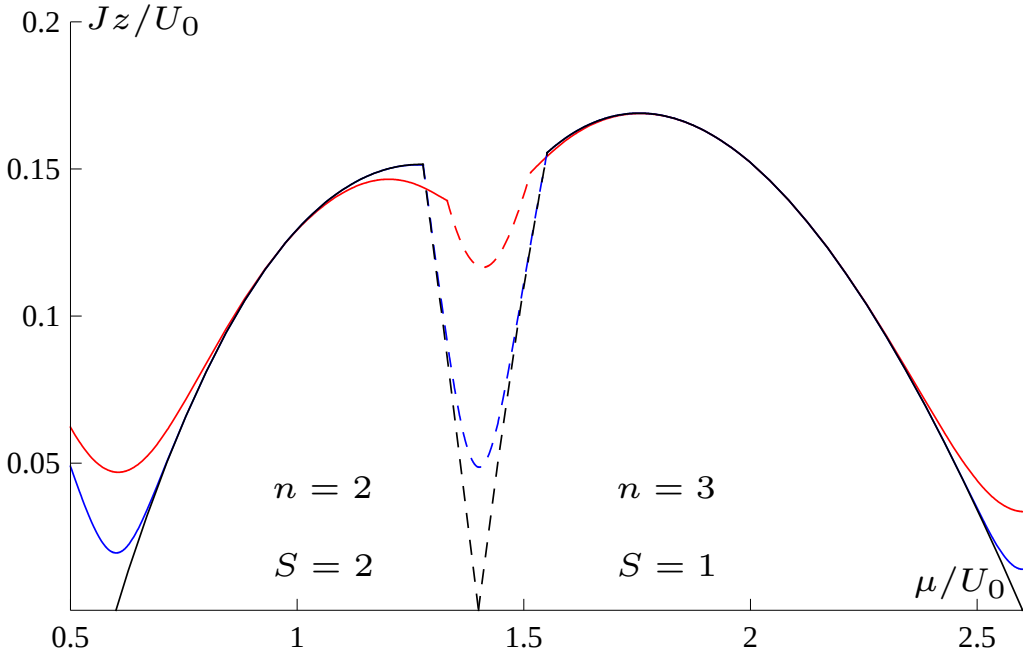

- Fully polarized gas ($\eta \gg U_2$) reproduces phase diagram of scalar BHM

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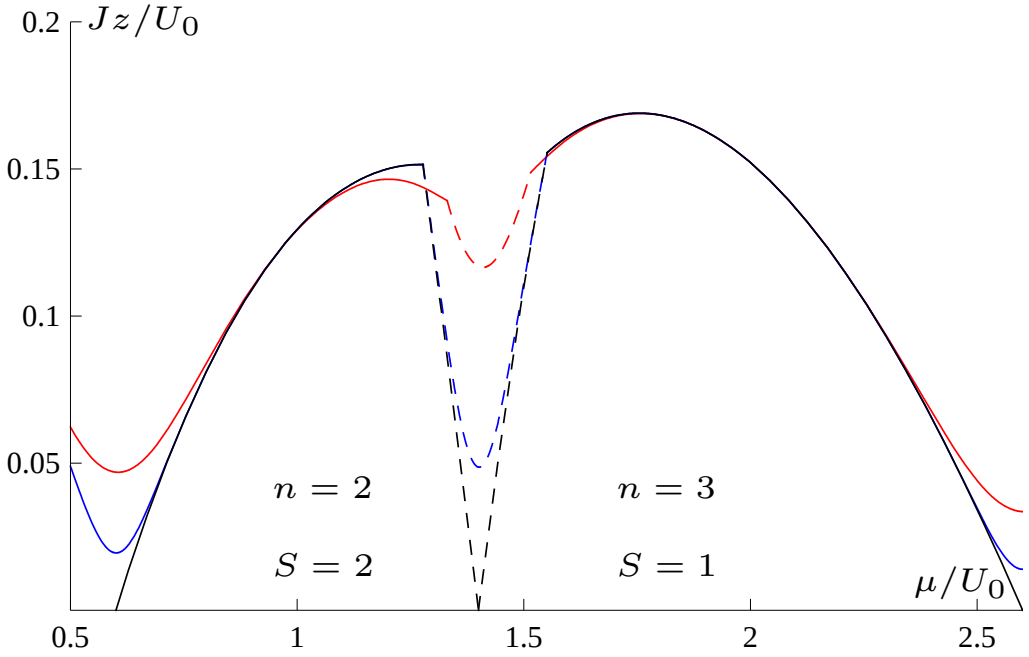

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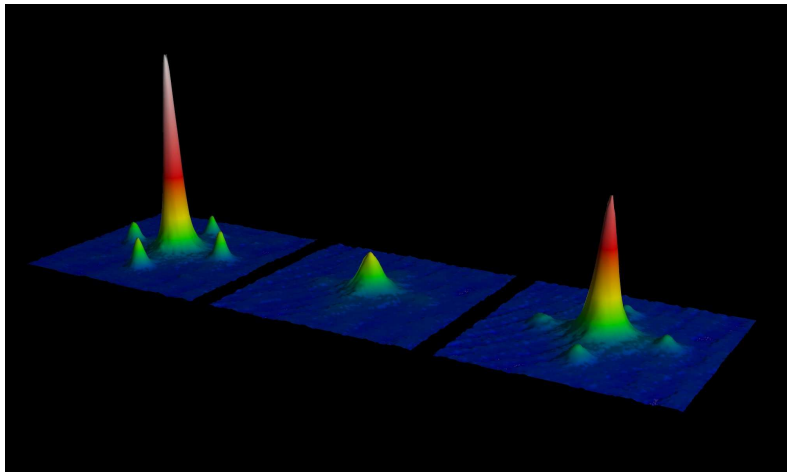
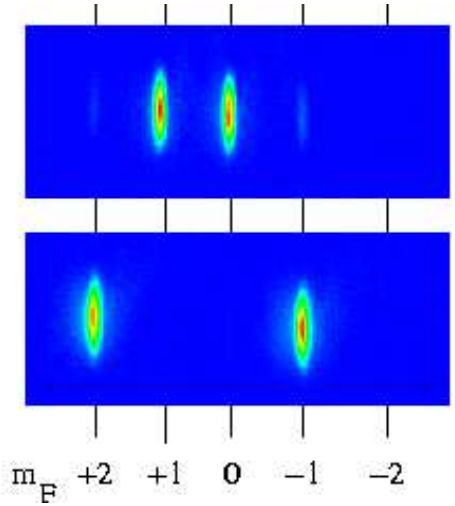
- Fully polarized gas ($\eta \gg U_2$) reproduces phase diagram of scalar BHM
- Ground state for $\eta = 0$:
  $\Phi_G^{(0)} = |0, 0, n\rangle$ (n even)
  $\Phi_G^{(0)} = |1, m, n\rangle$ (n odd)

  Threefold degeneracy, $\eta \to 0$ limit discontinuous

Time-Of-Flight Absorption Imaging



source: MIT, Ketterle group



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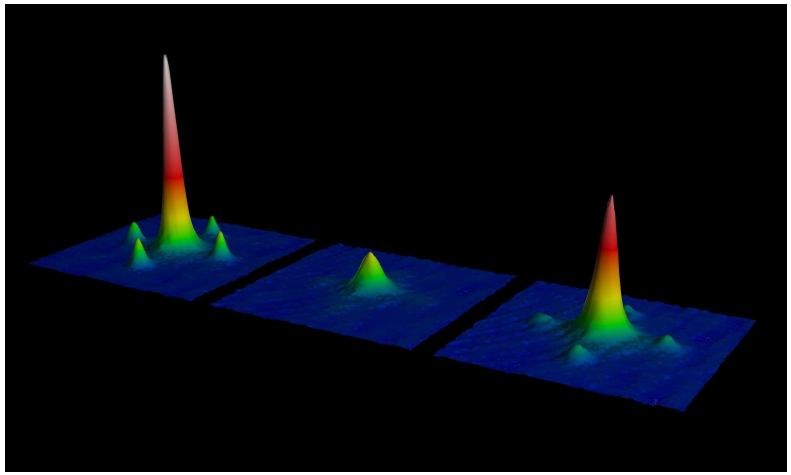

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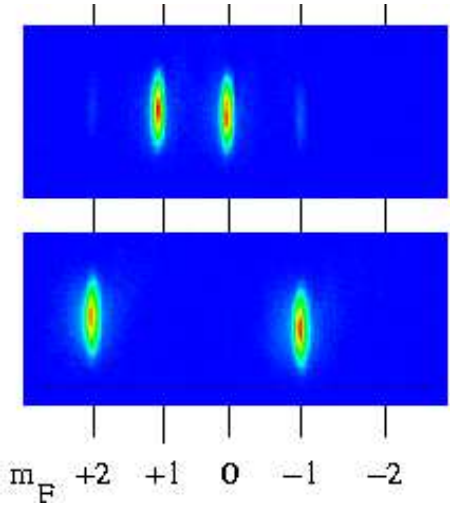

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- Time-of-flight measurements show momentum space distribution

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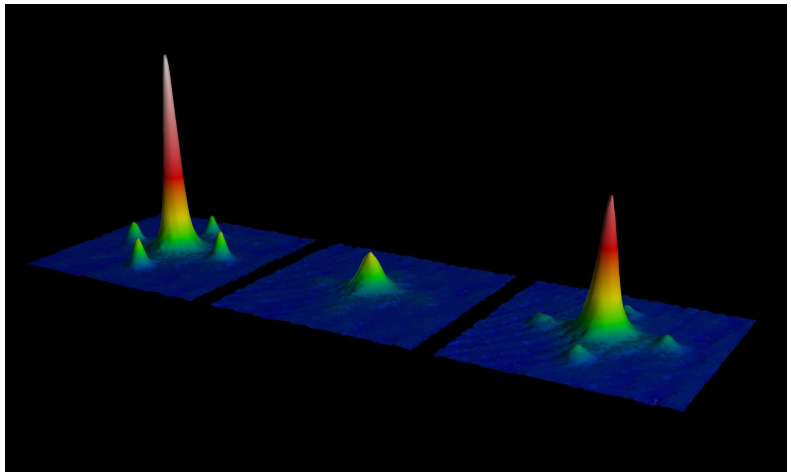

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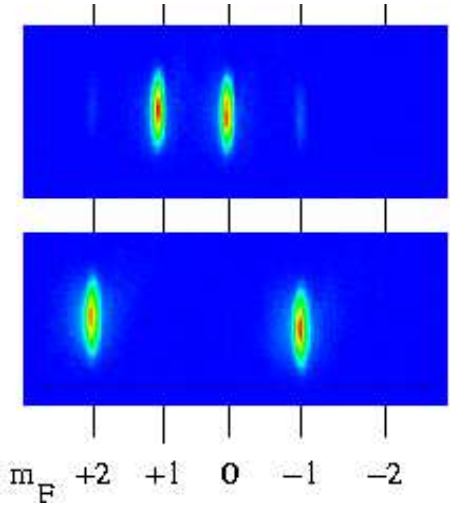

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- Time-of-flight measurements show momentum space distribution
- Different spin-components separable by inhomogeneous magnetic fields

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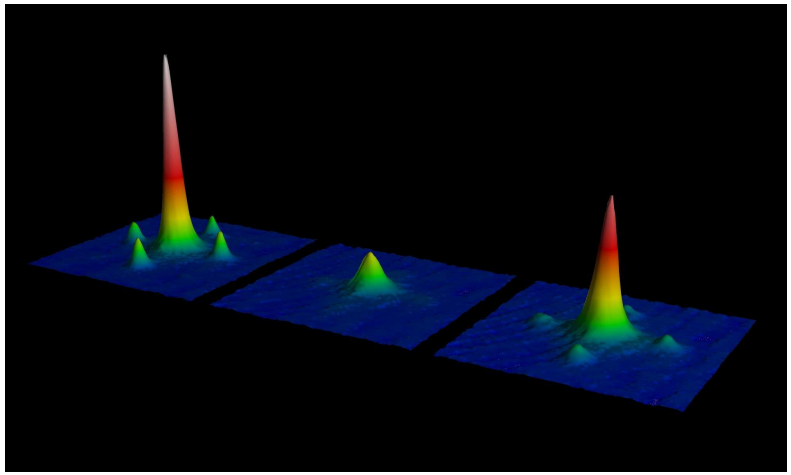

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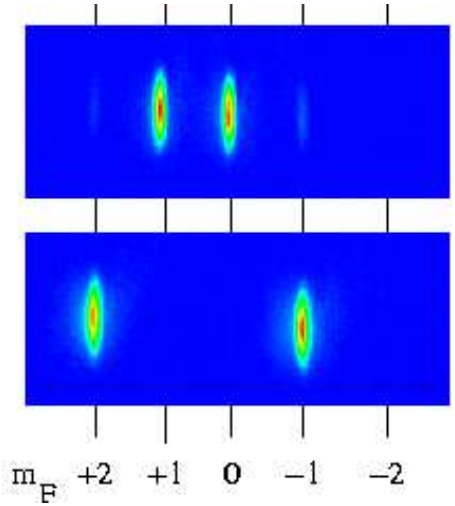

source: Universität Hamburg

- Time-of-flight measurements show momentum space distribution
- Different spin-components separable by inhomogeneous magnetic fields
- Calculation in BHM:

$$n(\mathbf{k}) = \sum_{\alpha} n_{\alpha}(\mathbf{k})$$

$$n_{\alpha}(\mathbf{k}) = |w(\mathbf{k})|^2 S_{\alpha}(\mathbf{k})$$

$$S_{\alpha}(\mathbf{k}) = \sum_{i,j} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \langle \hat{a}^{\dagger}_{i\alpha} \hat{a}_{j\alpha} \rangle$$

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$$\begin{aligned}\langle \hat{a}^\dagger_{i\alpha} \hat{a}_{j\alpha} \rangle =& \delta_{ij} n_\alpha + \delta_{d(i,j),1} 2JzC_\alpha + O(J^2) \\ C_\alpha =& \frac{M^2_{\alpha,S,m,n} O^2_{\alpha,S,m,n}}{U_0 + (2S+2)U_2} + \frac{M^2_{\alpha,S,m,n} P^2_{\alpha,S,m,n}}{U_0 + U_2} + \frac{N^2_{\alpha,S,m,n} O^2_{\alpha,S,m,n}}{U_0 + U_2} \\ &+ \frac{N^2_{\alpha,S,m,n} P^2_{\alpha,S,m,n}}{U_0 - 2SU_2}, \quad n_\alpha = O^2_{\alpha,S,m,n} + P^2_{\alpha,S,m,n}\end{aligned}$$

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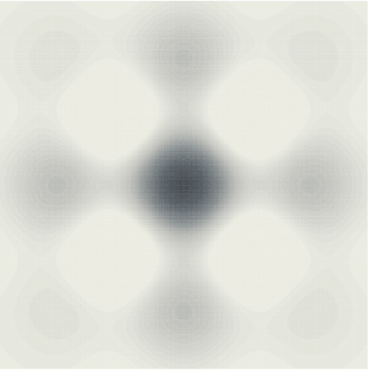
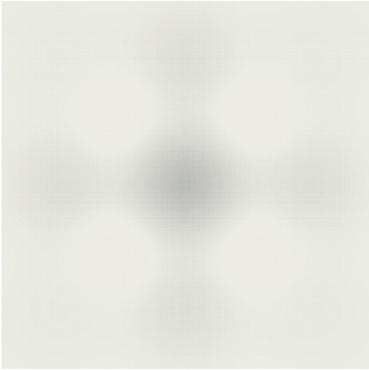
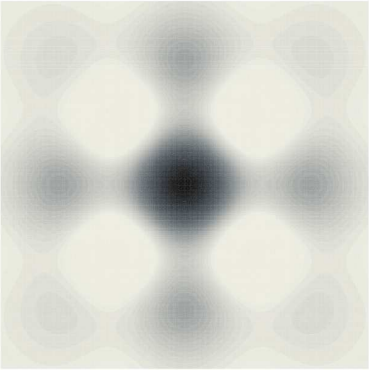
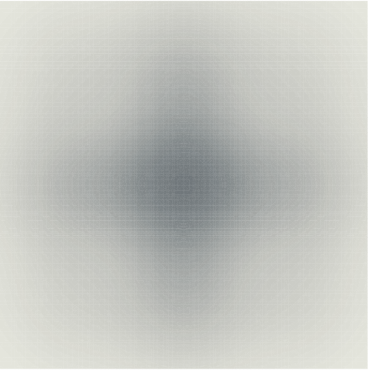
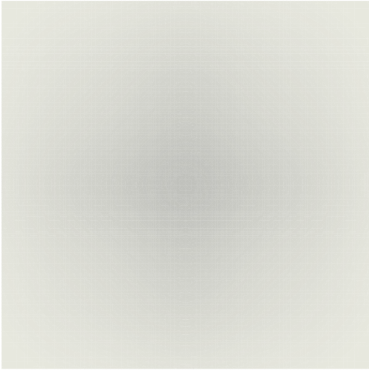
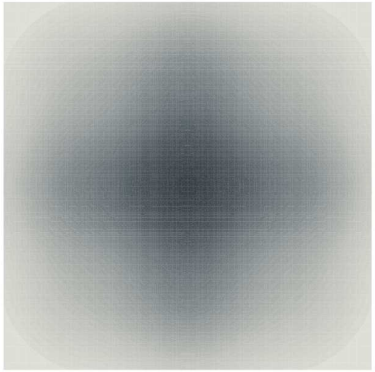
- Fully polarized gas $\Phi_G^{(0)} = |n, n, n\rangle$ yields $n_0(\mathbf{k}) = n_{-1}(\mathbf{k}) = 0$. $n_1(\mathbf{k})$ reproduces result of scalar BHM

Pictures

$\alpha = 1$	$\alpha = 0$	$\alpha = -1$	total
			
			

$U_2 = 0.04\,U_0$, $n = 3$, $S = 1$. $V_0 = 8\,E_R$ (1st line), $V_0 = 14\,E_R$ (2nd line)

Momentum space correlations

- Hopping leads to correlation between different sites

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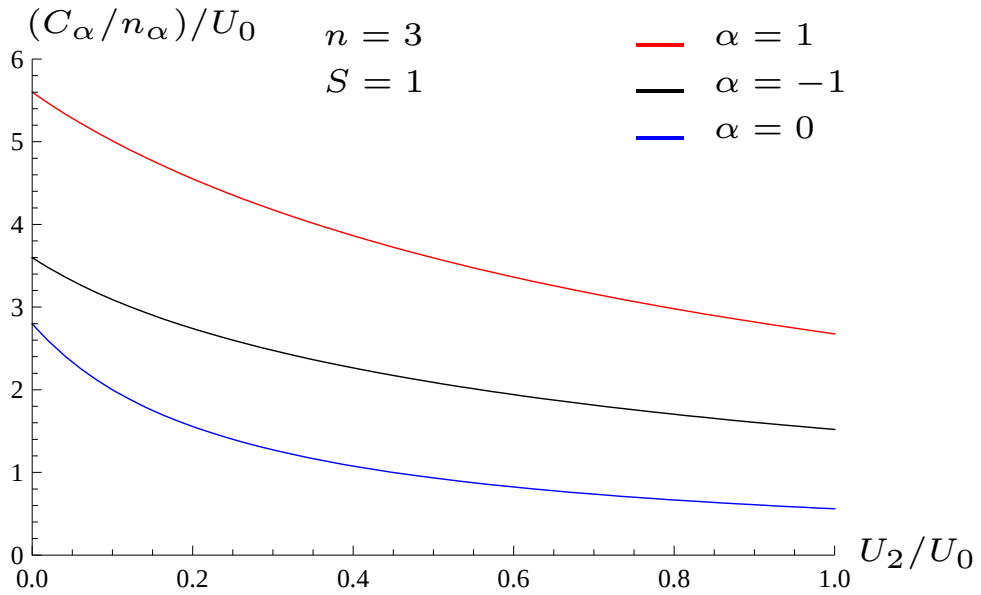
- Different hyperfine components behave slightly different

Momentum space correlations

- Hopping leads to correlation between different sites
- Different hyperfine components behave slightly different
- Qualitative measure of correlations: C_α/n_α
  connection to visibility



Outlook

- Phase Transition:
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  - Order of phase transition
  - Quantum corrections to mean-field result
  - Different phases within one Mott-lobe
  - Taking dipolar interaction between particles into account

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- Time-of-Flight
  - Further quantitative analysis: visibility
  - Extension to triangular optical lattice to study frustration effects