Quantum Phases of a Multi-component Bose Gas in an Optical Lattice

K. Ziegler, Augsburg *

- One-component Bose Gas:
  BEC ⟷ Mott insulator
- Two-component Bose Gas:
  "magnetic" phases
- N-component Bose Gas:
  exactly soluble Models

* with Ch. Moseley
C. Ates

Motivation: condensed matter phys.

phases and phase transitions in a

Fermi gas: ($\approx 10^{23}$ particles)

- Mott insulator } MIT
- metal } MIT
- superconductor
- magnetic phases
- orbital phases ("orbital order")
- flux phases (?)
- phases related to disorder
  (Anderson local.)
  (glass phases)

Bose gas: ($\approx 10^4 \ldots 10^7$ particles)

- BE condensate

Quantum Phases in a Bose Gas

Bose-Einstein Condensate

phase coherent state:

$$\langle a_{rt} a^{\dagger}_{r't'} \rangle \neq 0$$

local particle number fluctuates

Mott Insulator

phase fluctuates incoherently (gap)

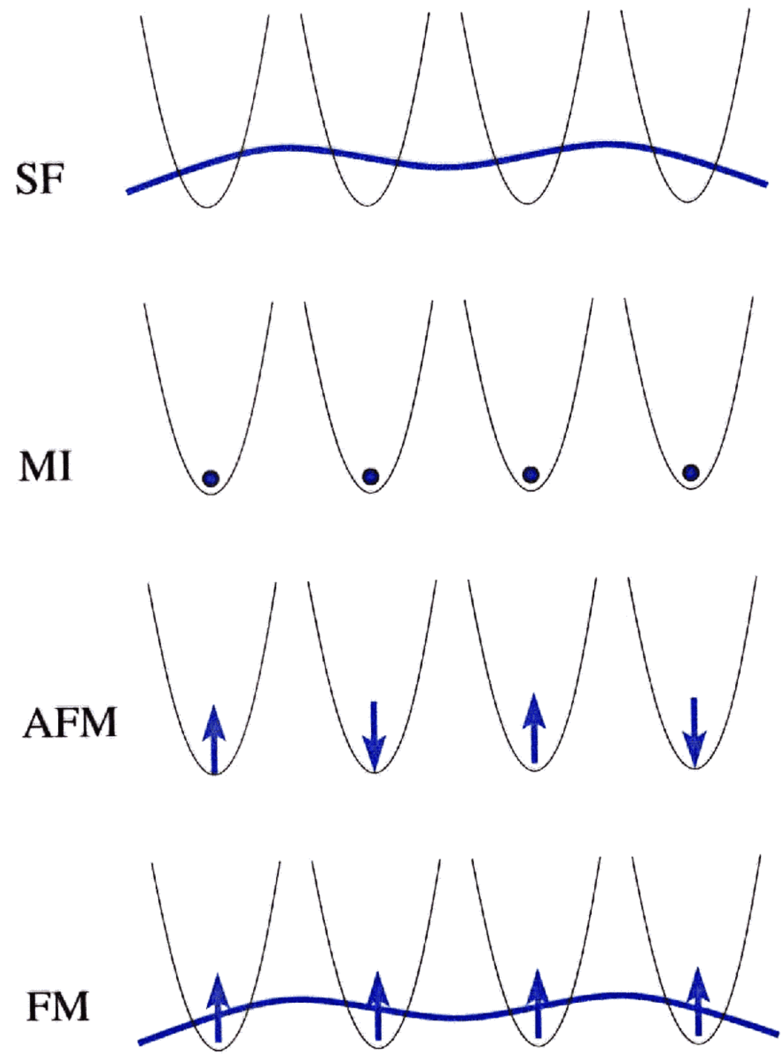
local particle number is fixed:

$$\langle a^{\dagger}_{rt} a_{rt} \rangle = \text{integer}$$

Spin-Ordered State

spin is correlated:

$$\langle a_{rt\sigma} a^{\dagger}_{rt\sigma} - a_{rt\sigma'} a^{\dagger}_{rt\sigma'} \rangle \neq 0 \quad (\sigma' \neq \sigma)$$



One-component Bose Gas

a) Bose-Hubbard Model: $H = H_0 + H_1$

$$H_0 = \sum_{\mathbf{r}} [-\mu n_{\mathbf{r}} + U n_{\mathbf{r}}(n_{\mathbf{r}} - 1)] \ , \quad n_{\mathbf{r}} = a_{\mathbf{r}}^\dagger a_{\mathbf{r}}$$

$$H_1 = -t \sum_{<\mathbf{r},\mathbf{r}'>} a_{\mathbf{r}}^\dagger a_{\mathbf{r}'}$$

b) Hard-core Bose Gas (projection to $n_{\mathbf{r}} = 0, 1$):

$$H_{hcb} = -t \sum_{<\mathbf{r},\mathbf{r}'>} A_{\mathbf{r}}^\dagger A_{\mathbf{r}'} - \mu \sum_{\mathbf{r}} A_{\mathbf{r}}^\dagger A_{\mathbf{r}} \quad ({A^\dagger}^2 = 0)$$

One-component Bose Gas

Hamiltonian:

$$H = \int \Big(\frac{\hbar^2}{2m} \nabla\Psi^\dagger \nabla\Psi + V\Psi^\dagger\Psi\Big) d^3r + \frac{1}{2} U \int \Psi^\dagger\Psi^\dagger\Psi\Psi d^3r$$

Dilute Bose gas

mean-field theory: wave function $\Psi_{MF}(r_1, r_2, ..., r_N) = \prod_j \Psi_0(r_j)$

$$\langle H \rangle_0 = N \int \Big(\frac{\hbar^2}{2m} |\nabla\Psi_0|^2 + V|\Psi_0|^2\Big) d^3r + \frac{N(N-1)}{2} U \int |\Psi_0|^4 d^3r$$

minimization yields the Gross-Pitaevskii Eq.:

$$\Big(-\frac{\hbar^2}{2m}\nabla^2 + V + NU|\Psi_0|^2\Big)\Psi_0 = \mu\Psi_0$$

μ: Lagrange multiplier for the normalization of Ψ_0

Lattice Systems

Grand-canonical Ensemble

$$Z = Tre^{-\beta H}$$

Hard-core Bosons:

Mean-field Approximation: $|\Psi_{MF}\rangle = \prod_{\mathbf{r}} \left[\cos\eta_{\mathbf{r}} + e^{i\psi_{\mathbf{r}}}\sin\eta_{\mathbf{r}} A^\dagger_{\mathbf{r}}\right]|0\rangle$

$$\langle\Psi_{MF}|H_{hcb}|\Psi_{MF}\rangle = -\sin^2\eta\left[t\cos^2\eta \sum_{<\mathbf{r},\mathbf{r}'>} \cos(\psi_{\mathbf{r}} - \psi_{\mathbf{r}'}) + \sum_{\mathbf{r}} \mu\right]$$

ground state: $\cos(\psi_{\mathbf{r}} - \psi_{\mathbf{r}'}) = 1$

$$\sin^2\eta = \begin{cases} 0 & \text{for } \mu \le -2dt \\ 1/2 + \mu/4dt & \text{for } -2dt < \mu < 2dt \\ 1 & \text{for } 2dt \le \mu \end{cases}$$

Spin-1/2 Representation of the Hard-core Bose Gas

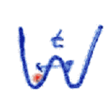
$$S^x = (A + A^\dagger)/2, \quad S^y = i(A - A^\dagger)/2, \quad S^z = A^\dagger A - 1/2$$

XY model with a magnetic field in z direction:

$$H_{hcb} = -t \sum_{<\mathbf{r},\mathbf{r}'>} (S^x_{\mathbf{r}} S^x_{\mathbf{r}'} + S^y_{\mathbf{r}} S^y_{\mathbf{r}'}) - \mu \sum_{\mathbf{r}} S^z_{\mathbf{r}}$$

Grand-canonical Ensemble with Two Sites

$$|\Psi_0\rangle = \begin{cases} |0,0\rangle & \text{for } \mu < -t \\ (|0,1\rangle + |1,0\rangle)/\sqrt{2} & \text{for } -t < \mu < t\,. \\ |1,1\rangle & \text{for } \mu > t \end{cases}$$



Two-component Bose-Hubbard Model

$$H_0 = \sum_{\mathbf{r}} [-\mu n_{\mathbf{r}} + U n_{\mathbf{r}}(n_{\mathbf{r}} - 1)] \quad , n_{\mathbf{r}} = a^\dagger_{\mathbf{r},\uparrow} a_{\mathbf{r},\uparrow} + a^\dagger_{\mathbf{r},\downarrow} a_{\mathbf{r},\downarrow}$$

$$H_1 = - \sum_{<\mathbf{r},\mathbf{r}'>} \sum_{\sigma,\sigma'} t_{\sigma,\sigma'} a^\dagger_{\mathbf{r},\sigma} a_{\mathbf{r}',\sigma'}$$

ground states for $N = 0, 1$ particles:

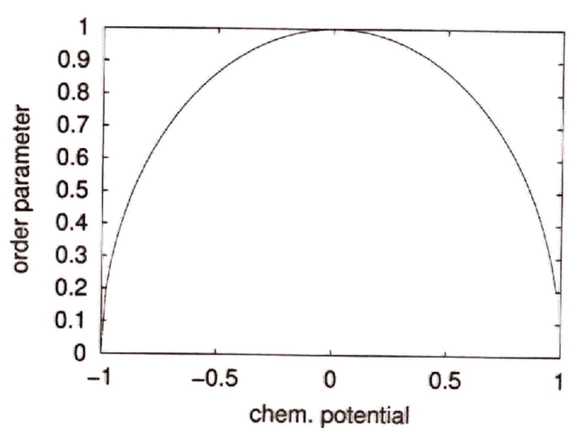
$$|\Psi_0\rangle = \begin{cases} |0,0\rangle & \text{for } \mu < -t \\ (|0,\uparrow\rangle + |\uparrow,0\rangle)/\sqrt{2}, \quad (|0,\downarrow\rangle + |\downarrow,0\rangle)/\sqrt{2} & \text{for } -t < \mu < t \end{cases}$$

$-t < \mu < t$: (degenerate) ferromagnetic states

degeneracy can be lifted by an infinitesimal magnetic field

Superfluid Order Parameter

$$\langle \Psi_{MF} | A_{\mathbf{r}} | \Psi_{MF} \rangle = e^{i\psi_{\mathbf{r}}} \cos\eta \sin\eta$$



Continued Fraction of the Projected System

Hilbert space for a lattice with N sites and N particles

If P_{2k} projects on states with k pairs of empty/doubly-occpied sites The resolvent

$$P_0(z - iH)^{-1}P_0 \tag{1}$$

satisfies the recurrence relation ($k \geq 0$):

$$P_{2k}(z - iH)^{-1}_{2k-1}P_{2k} = (P_{2k}(z - iH)P_{2k} + P_{2k}HP_{2k+2}(z - iH)^{-1}_{2k+1}P_{2k+2}HP_{2k})^{-1}_{2k}$$

1) Iteration yields continued-fraction representation of (1)

2) Truncation of the CFR gives effective Hamiltonian

$$P_0(z - iH)^{-1}P_0 \approx (z - iH_{eff})^{-1}_0$$

Effective Hamiltonian

$$H_{eff} = -((\Delta E)^2 + P_0H_1^2P_0)^{1/2}, \quad \Delta E = [E(0) + E(2)]/2 - E(1) = U$$

two-component Bose-Hubbard model (NO spin flip):

hard-core Bose representation:

$$-P_0H_1^2P_0 = -\sum_{<\mathrm{r},\mathrm{r}'>}\left[t_\uparrow t_\downarrow A^\dagger_\mathrm{r}A_{\mathrm{r}'} + \frac{t_\uparrow^2 + t_\downarrow^2}{2}(1 - A^\dagger_\mathrm{r}A_\mathrm{r})A^\dagger_{\mathrm{r}'}A_{\mathrm{r}'}\right]$$

$|\downarrow\rangle \to |0\rangle$
$|\uparrow\rangle \to |1\rangle$

spin-1/2 representation:

$$-t_\uparrow t_\downarrow \sum_{<\mathrm{r},\mathrm{r}'>}\left[S^x_\mathrm{r}S^x_{\mathrm{r}'} + S^y_\mathrm{r}S^y_{\mathrm{r}'}\right] + \frac{t_\uparrow^2 + t_\downarrow^2}{2}\sum_{<\mathrm{r},\mathrm{r}'>}S^z_\mathrm{r}S^z_{\mathrm{r}'}$$

Mean-field Approximation

a) Product ansatz:

$$|\Psi_{MF}\rangle = \prod_{\mathbf{r}} \left[\cos\eta_{\mathbf{r}} + e^{i\psi_{\mathbf{r}}}\sin\eta_{\mathbf{r}} A_{\mathbf{r}}^\dagger\right]|0\rangle$$

$$-\langle\Psi_{MF}|P_0 H_1^2 P_0|\Psi_{MF}\rangle =$$

$$-\sum_{<\mathbf{r},\mathbf{r}'>}\left(t_\uparrow t_\downarrow \cos(\psi_{\mathbf{r}}-\psi_{\mathbf{r}'})\cos\eta_{\mathbf{r}}\sin\eta_{\mathbf{r}}\cos\eta_{\mathbf{r}'}\sin\eta_{\mathbf{r}'} + \frac{t_\uparrow^2+t_\downarrow^2}{2}\cos^2\eta_{\mathbf{r}}\sin^2\eta_{\mathbf{r}'}\right)$$

uniform solution: $|\Psi\rangle_h$: $\sin^2\eta_{\mathbf{r}} = \cos^2\eta_{\mathbf{r}'} = 1/2$

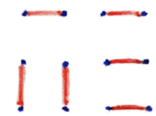
staggered solution: $|\Psi\rangle_i$: $\sin^2\eta_{\mathbf{r}} = 1, \quad \cos^2\eta_{\mathbf{r}'} = 1$

ground-state energies: $E_i \le E_h$ ('=' for $t_\uparrow = t_\downarrow$)

superfluid order parameter: $\langle\Psi_{MF}|a_{\mathbf{r}}|\Psi_{MF}\rangle_h = 0$

spin order parameter: $\langle\Psi_{MF}|A_{\mathbf{r}}|\Psi_{MF}\rangle_h = \langle\Psi_{MF}|a_{\mathbf{r},\downarrow}^\dagger a_{\mathbf{r},\uparrow}|\Psi_{MF}\rangle_h = e^{i\psi_{\mathbf{r}}}\cos\eta_{\mathbf{r}}\sin\eta_{\mathbf{r}}$

b) Dimerized ansatz:



$$|\Psi_D\rangle = \prod_{<\mathbf{r},\mathbf{r}'>\in D} \frac{1}{\sqrt{2}}(e^{i\varphi_{\mathbf{r}}}A_{\mathbf{r}}^\dagger + e^{i\varphi_{\mathbf{r}'}}A_{\mathbf{r}'}^\dagger)|0\rangle$$

where D is a set of dimers $\{<\mathbf{r},\mathbf{r}'>\}$.

$$-\langle\Psi_D|P_0 H_1^2 P_0|\Psi_D\rangle = -\frac{t_\uparrow t_\downarrow}{2}\sum_{<\mathbf{r},\mathbf{r}'>\in D}\cos(\varphi_{\mathbf{r}}-\varphi_{\mathbf{r}'}) - \frac{t_\uparrow^2+t_\downarrow^2}{4}\sum_{<\mathbf{r},\mathbf{r}'>}$$

ground state energies: $E_D \le E_i \le E_h$ (first '=' for $t_\uparrow t_\downarrow = 0$)

superfluid order parameter: $\langle\Psi_D|a_{\mathbf{r}}|\Psi_D\rangle = 0$

spin order parameter: $\langle\Psi_D|A_{\mathbf{r}}|\Psi_D\rangle = 0 \quad \longrightarrow$ spin liquid ?

N-Component Bose Gas

1) without spin flip

$$H = -\frac{t}{N}\sum_{\langle r,r'\rangle}\sum_{z=1}^{N^2} A^+_{rz} A_{r'z}$$

(particles "carry spin" z)

Bose operator:

$$A^+_z A^+_{z'} = A^+_{\alpha\beta} A^+_{\alpha'\beta'} = (1-\delta_{\alpha\alpha'})(1-\delta_{\beta\beta'}) A^+_{\alpha\beta} A^+_{\alpha'\beta'}$$

2) with spin flip

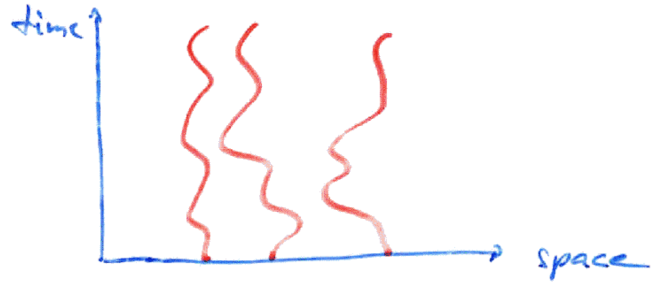
$$H = -\frac{t}{N}\sum_{\langle r,r'\rangle}\sum_{z,z'=1}^{N} A^+_{rz} A_{r'z'}$$

Bose operator:

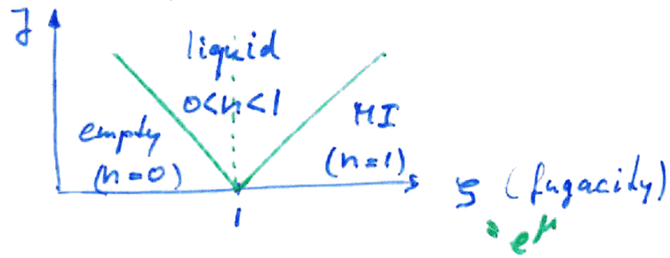
$$A^+_z A^+_{z'} = (1-\delta_{zz'}) A^+_z A^+_{z'}$$

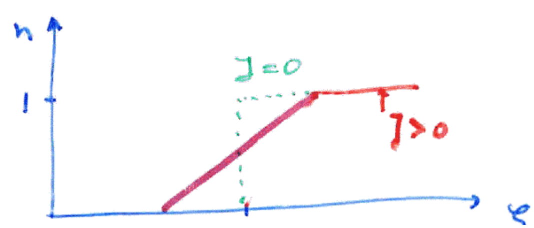
Hard-Core Bosons in $d=1$

1D HC Bosons $\xrightarrow[\text{principle}]{\text{Pauli}}$ 1D free fermions



T=0-phase diagram





Statistics $d \geq 3$

hard-core interaction $\leftrightarrow$ Pauli principle

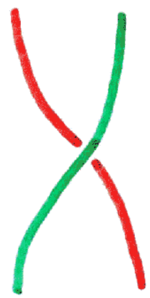
Problem: Exchange of two particles

wave function:

bosons

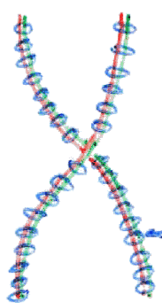
$+1$

fermions



-1

pairs of fermions



$(-1)^2 = +1$

gauge field

Effective Field Theories

$Z = \mathrm{Tr}\, e^{-\beta H}$

1) without spin flip: $u_{xx'}$: real matrix field

$$Z = \int \exp\left\{-N\left[\sum_{x,x'} \frac{(u_{xx'})^2}{g v_{xx'}} - 2 \log\det(1+u)\right]\right\} \mathcal{D}[u]$$

symmetry: $u \to O u O^T$

2) with spin flip: φ_x, χ_x: complex scalar field

$$Z = \int \exp\left\{-N\left[(\varphi, (1+w)^{-1}\varphi^*) + (\chi, \chi^*) - \sum_x \log\left(g^{-1}(\varphi_x + i\chi_x)(\varphi_x^* + i\chi_x^*)\right)\right]\right\} \mathcal{D}[\varphi, \chi]$$

symmetry: $U(1)$: $\left.\begin{matrix}\varphi_x \to e^{i\alpha}\varphi_x \\ \chi_x \to e^{i\alpha}\chi_x\end{matrix}\right\}$

1) and 2) agree for $N=1$.

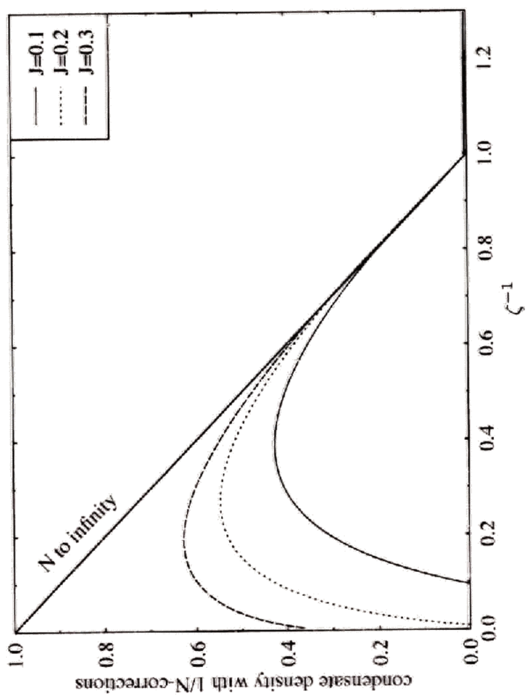
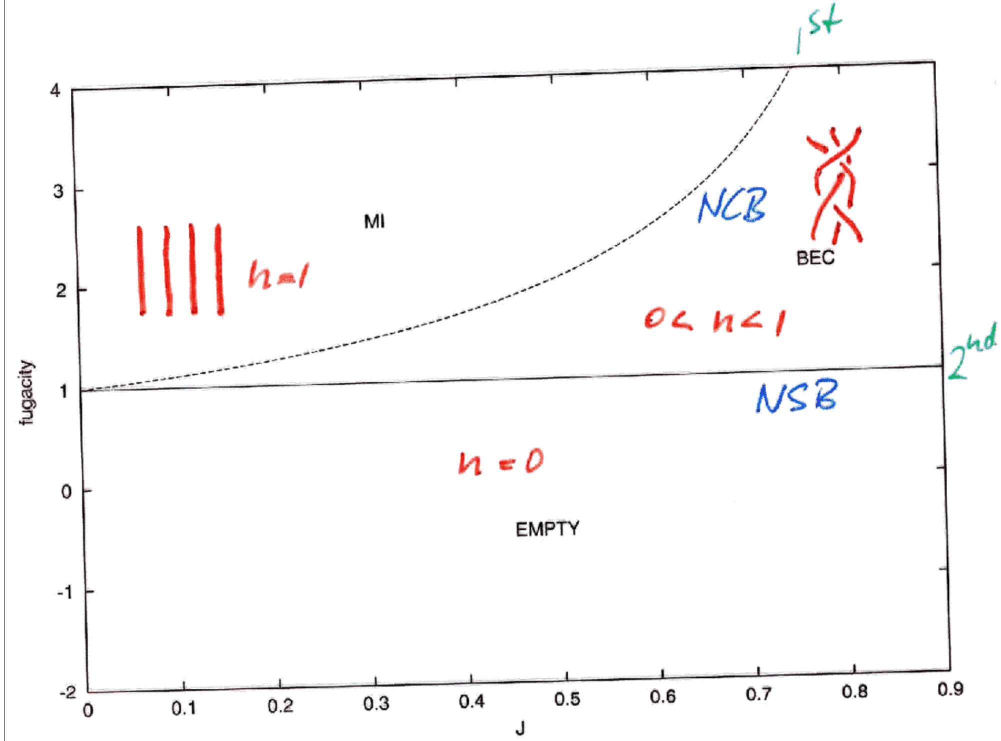


Figure 1: Condensate density at $N = 5$. The (positive) corrections to the total density are small compared to n_0.

$T = 0$–Phase Diagram



Spin Order $N \sim \infty$

1) without spin flip

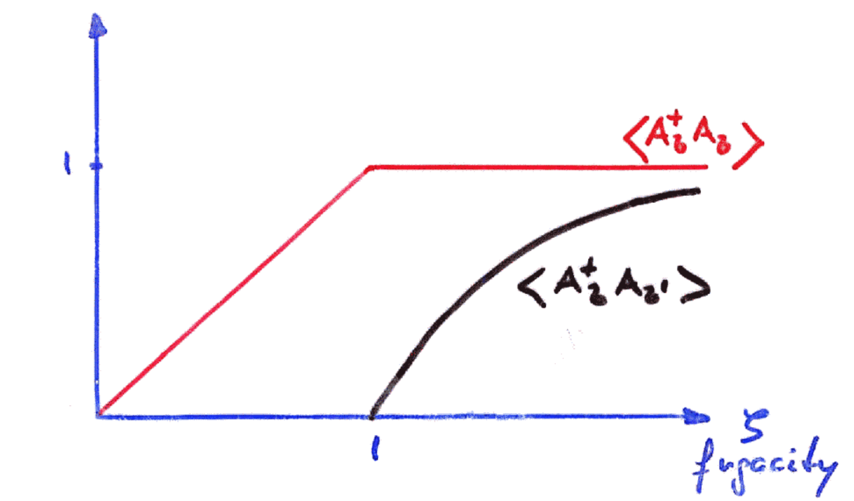
$$\langle A_z^+ A_{z'} \rangle \sim \zeta \delta_{zz'} \quad (\text{Mott insulator})$$

2) with spin flip

$$\langle A_z^+ A_z \rangle \sim \begin{cases} \zeta & \zeta < 1 \\ 1 & \zeta \geq 1 \end{cases}$$

$z \neq z'$:

$$\langle A_z^+ A_{z'} \rangle \sim \begin{cases} 0 & \zeta < 1 \\ 1 - 1/\zeta & \zeta \geq 1 \end{cases}$$



Conclusions

a Bose gas provides a wide range of phenomena depending on density, external potentials and internal degrees of freedom

dilute Bose gas:
Gross-Pitaevskii Equation: BE condensation incl. vortices

Bose gas in an optical lattice:
Bose-Hubbard model or hard-core Bose gas: quantum statistics phase transition to a Mott insulator

multi-component Bose gas:
"correlation" physics: complex spin structures