From the Bose-Hubbard model over disorder to the Bose-Fermi-Hubbard model:

a short introduction to cold bosons (and fermions)

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introduction

- want to consider ultracold atoms in optical lattice

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- working frame:
  - 2nd quantization
  - short range interaction (δ-like)
  - low energy regime ($\Rightarrow$ only lowest Bloch band occupied)
  - choose Wannier basis

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- want to consider ultracold atoms in optical lattice
- working frame:
  - 2nd quantization
  - short range interaction (δ-like)
  - low energy regime ($\Rightarrow$ only lowest Bloch band occupied)
  - choose Wannier basis
- study resulting effective Hamiltonian:
  - include addional species
  - change interaction (for instance site-to-site interaction)
  - introduce disorder

Bose-Hubbard model

Simplest model for interacting bosons in optical lattice

the (pure) Bose-Hubbard model

$$\widehat{\mathcal{H}} = -J_B \sum_{\langle ij \rangle} \widehat{a}_i^\dagger \widehat{a}_j + \frac{U}{2} \sum_i \widehat{n}_i(\widehat{n}_i - 1) - \mu_B \sum_i \widehat{n}_i$$

J_B: nearest neighbour hopping amplitude

U: on-site interaction

μ_B: chemical potential

We are interested in the (μ_B, J_B)-phase diagram

vanishing hopping $J_B/U \to 0$

BHM Hamiltonian decouples sites and can be rewritten:

$$\widehat{\mathcal{H}} = \sum_i \frac{U}{2}(\widehat{n}_i - \bar{n})^2 + const$$

with $\bar{n} = \frac{1}{2} + \frac{\mu}{U}$

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Mott insulator

All sites have the same groundstate with $n_0 = \lfloor \bar{n} \rfloor$ bosons

exception: degenerate groundstate if $\mu \in \mathbb{Z}$

vanishing interaction $J_B/U \longrightarrow \infty$

resulting in free bosons (solution via Fourier transform):

$$\widehat{\mathcal{H}} = -2J_B \sum_k \cos(k)\, \widehat{f}_k^\dagger \widehat{f}_k - \mu_B \sum_k \widehat{f}_k^\dagger \widehat{f}_k$$

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superfluid phase

coherent ground state (spread over the whole lattice)

solution: filled fermi sea

summary: phase properties (1D)

Mott insulator

- fixed atom number per site
- rapidly decaying correlations (exponential decay)
- incompressible phase ($\kappa = \frac{\partial \langle \widehat{n} \rangle}{\partial \mu_B} \equiv 0$)

summary: phase properties (1D)

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- rapidly decaying correlations (exponential decay)
- incompressible phase ($\kappa = \frac{\partial \langle \widehat{n} \rangle}{\partial \mu_B} \equiv 0$)

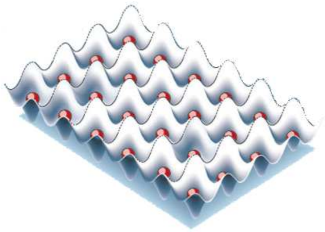
Superfluid

- atom number fluctuating
- slowly decaying correlations (algebraic decay)
- compressible phase ($\kappa = \frac{\partial \langle \widehat{n} \rangle}{\partial \mu_B} \neq 0$)

phase distinction - site occupation

Mott insulator

fixed atom number per site



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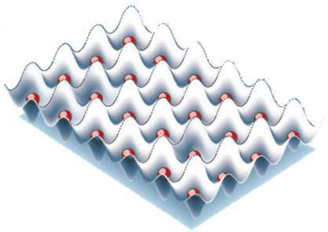
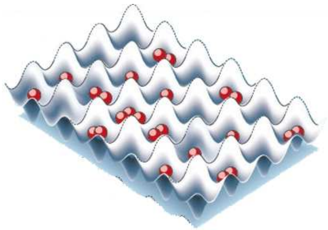


Superfluid

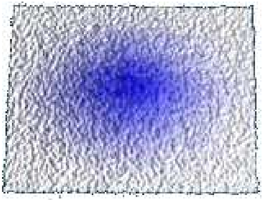
atom number per site fluctuating



phase distinction - time of flight images

Mott insulator

exponential decay



$$\text{TOF-picture} = \mathcal{F}\left[\langle \widehat{a}_i^\dagger \widehat{a}_j \rangle\right]$$

phase distinction - time of flight images

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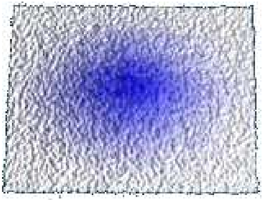
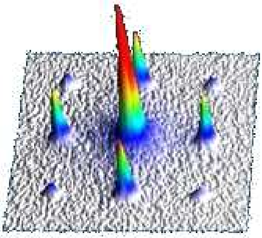


Superfluid

algebraic decay

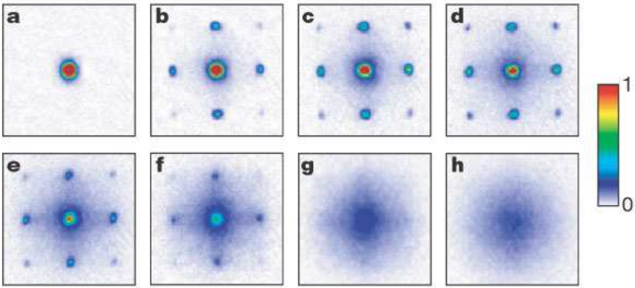


$$\text{TOF-picture} = \mathcal{F}\left[\langle \widehat{a}_i^\dagger \widehat{a}_j \rangle\right]$$

phase distinction - ramping of the lattice depth

Drive the transition by changing the depth of the lattice:

shallow



deep

theoretical approaches

theoretical approaches

- **mean field approach (2nd order)**
  - mimic influence of neighbouring sites by local parameter Ψ
  - this orderparameter gives phases: $\Psi \neq 0 \Rightarrow$ SF

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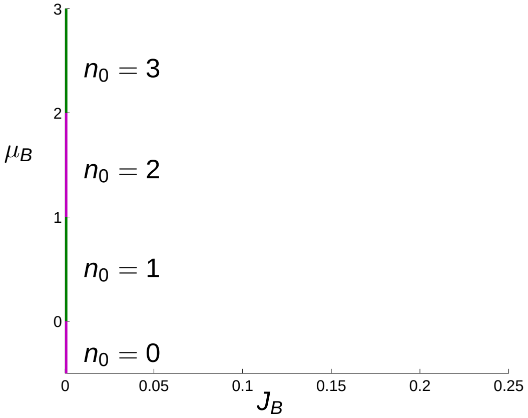
- **mean field approach (2nd order)**
  - mimic influence of neighbouring sites by local parameter Ψ
  - this orderparameter gives phases: $\Psi \neq 0 \Rightarrow$ SF
- **strong coupling expansion (3rd order)**
  - calculate energy of ground and exited (particle/hole) states by 3rd order degenerate perturbation theory
  - energy difference gives chemical potentials and therefore phase boundaries

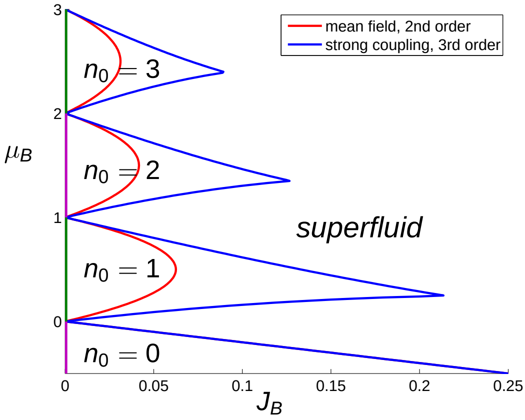
and finally: the phase diagram

First: remember the case $J_B = 0$



and finally the diagram

Second: now include the hopping



Bose-Hubbard model with disorder

What happens if we introduce disorder to the system?
Kinds of disorder:

- interaction disorder: $U \mapsto U_i$
- hopping disorder: $J \mapsto J_i (\mapsto J_{ij})$
- energy disorder: $\mu_B \mapsto \mu_i^B$

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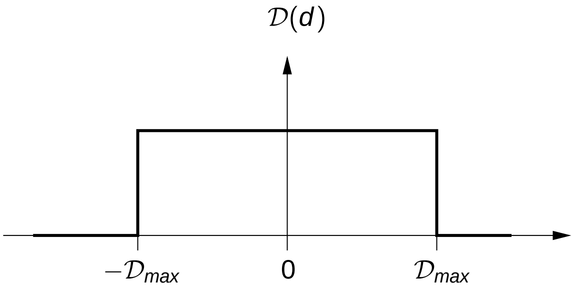
disordered Bose-Hubbard model

$$\widehat{\mathcal{H}} = -J_B \sum_{\langle ij \rangle} \widehat{a}_i^\dagger \widehat{a}_j + \frac{U}{2} \sum_i \widehat{n}_i (\widehat{n}_i - 1) - \sum_i (\mu_B + \delta_i) \widehat{n}_i$$

some notes on the disorder

consider a disorder distribution $\mathcal{D}(d)$ like:



distinguish small ($\mathcal{D}_{max} < U/2$) and large ($\mathcal{D}_{max} > U/2$) disorder

vanishing hopping $J_B/U \rightarrow 0$

superfluid phase

- compressible
- algebraicly decaying correlations
- ungapped
  (adding a additional boson to the system increases energy only infinitesimally)

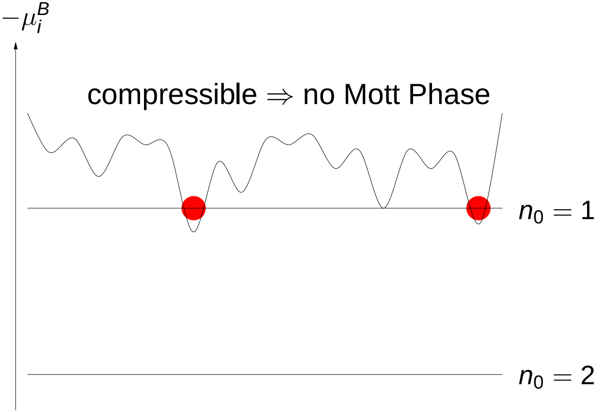
vanishing interaction $J_B/U \to \infty$

What is groundstate?

Answer is given by the questions:

- What happens if we again vary μ_B?
- What are the (energetically) allowed states?
- Is the phase incompressible?

an intuitive picture



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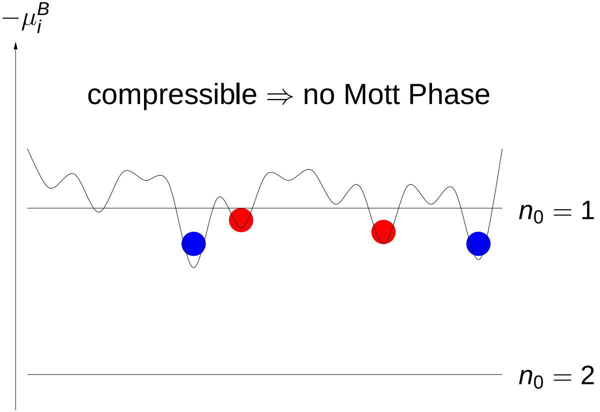

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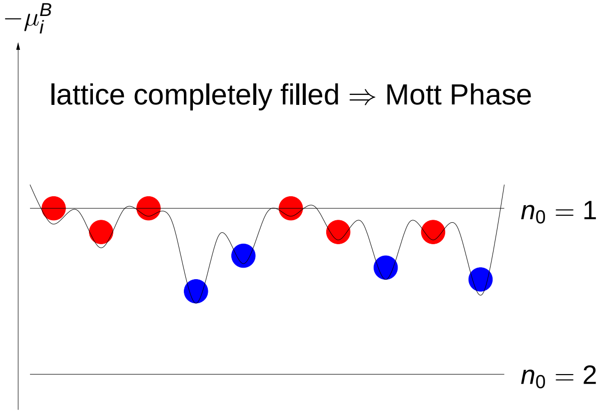

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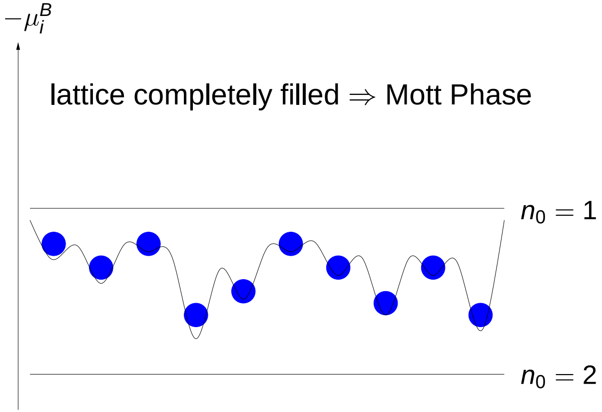

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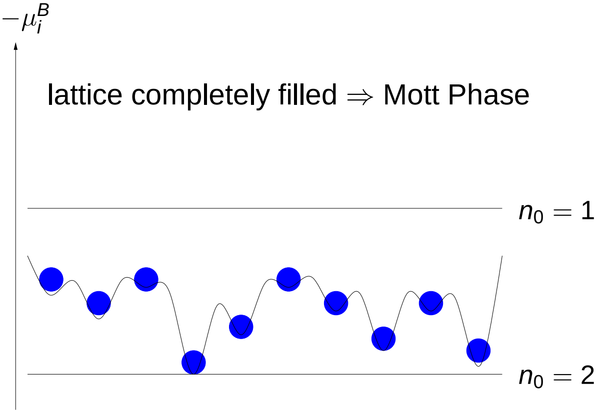
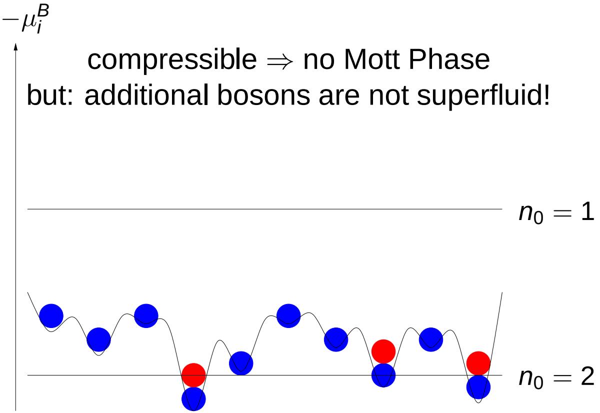


an intuitive picture

compressible $\Rightarrow$ no Mott Phase

but: additional bosons are not superfluid!



adding hopping

- Mott phases extend as usual with increasing hopping but vanish earlier
- superfluid is dominant at large hopping
- additional phase already appears at $J_B = 0$:

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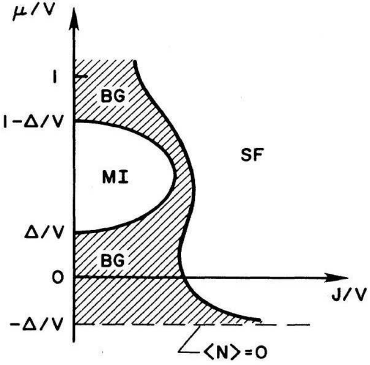
bose glas phase:

- fluctuating number of atoms per site
- compressible
- exponentially decaying correlations
- gapless

the phase diagram



from M.P.A. Fisher *et. al.*, Phys. Rev. B **40**, 546 (1988)

further remarks

- combines properties of Mott and superfluid phase:
  - decaying correlations like a Mott phase
  - compressible like a superfluid
- from TOF pictures industinguishable from Mott phase
- additionally measure the excitation spectrum

$\Rightarrow$ ungapped like a superfluid

Bose-Fermi-Hubbard model

- Now add polarized fermions to the system under same assumptions (Bloch band, Wannier states, ...)
- restrict to a fixed fermion density

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the Bose-Fermi-Hubbard model

$$\widehat{\mathcal{H}} = -J_F \sum_{\langle ij \rangle} \widehat{c}_i^\dagger \widehat{c}_j - J_B \sum_{\langle ij \rangle} \widehat{a}_i^\dagger \widehat{a}_j + \frac{U}{2} \sum_i \widehat{n}_i (\widehat{n}_i - 1)$$
$$- \mu_B \sum_i \widehat{n}_i + V \sum_i \widehat{n}_i \widehat{m}_i$$

$J_F = 0$: connection to disordered BHM

rewrite Hamiltonian:

the $J_F = 0$ Bose-Fermi-Hubbard model

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- presence of a fermion acts like disorder

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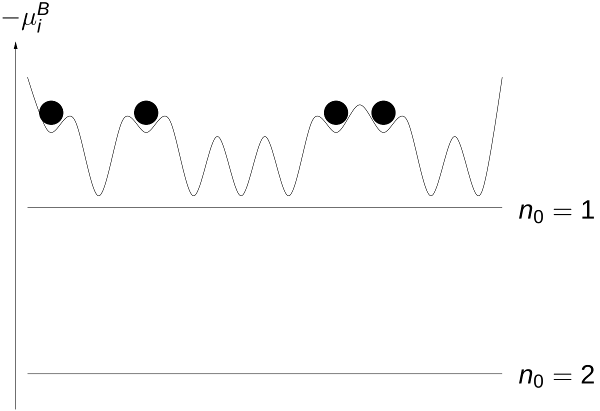
- presence of a fermion acts like disorder
- but a very special disorder distribution:

$$\mathcal{D}(d) = (1 - \rho_F)\delta(d) + \rho_F \delta(d - V)$$

$\Rightarrow$ different effects

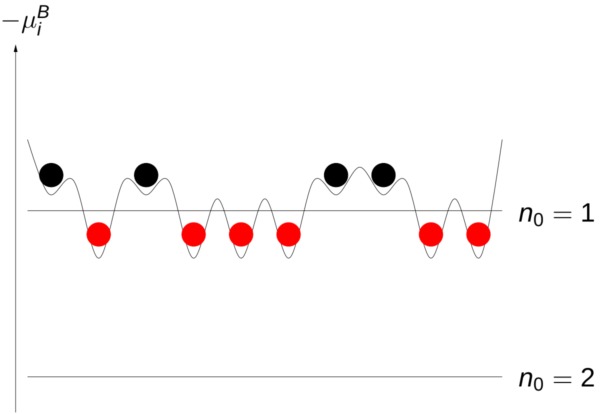
2nd intuitive picture

only (some) fermions, no bosons



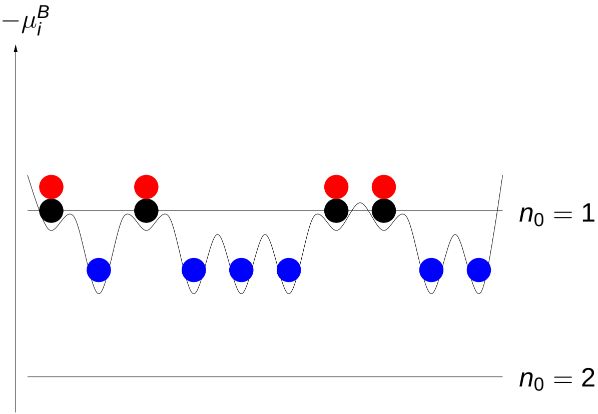
2nd intuitive picture

non fermion sites filled up $\Rightarrow$ incompressible but no Mott



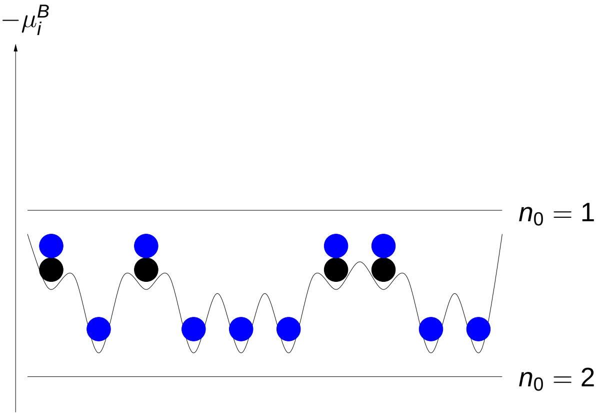
2nd intuitive picture

all sites filled up $\Rightarrow$ true Mott phase



2nd intuitive picture

Mott phase



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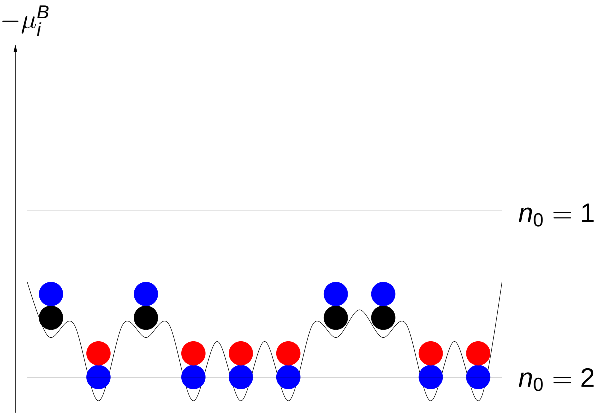
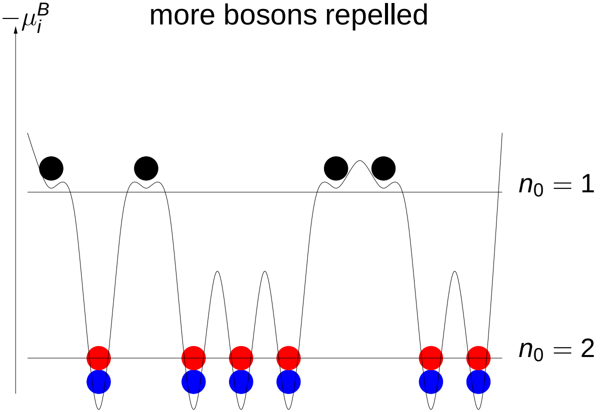


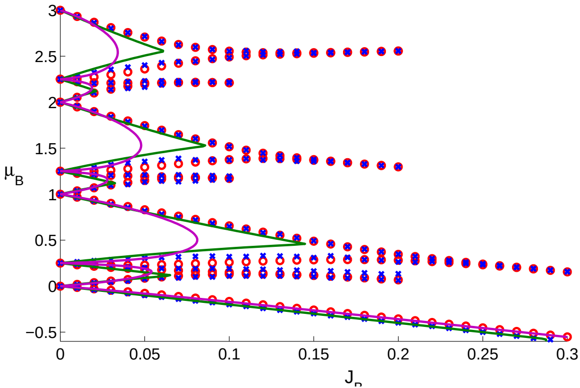
2nd intuitive picture

large V behave different:
more bosons repelled



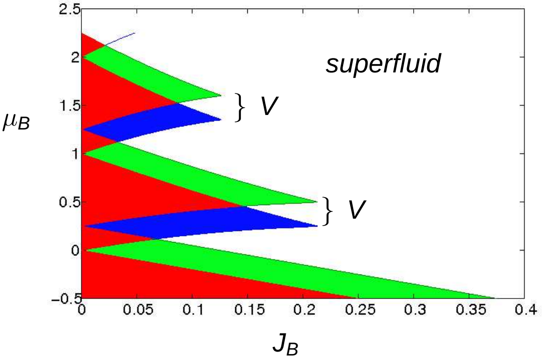
and fi nally the diagram

DMRG - calculation: $U = 1$, $V = 0.25$, $\rho_F = 0.25$



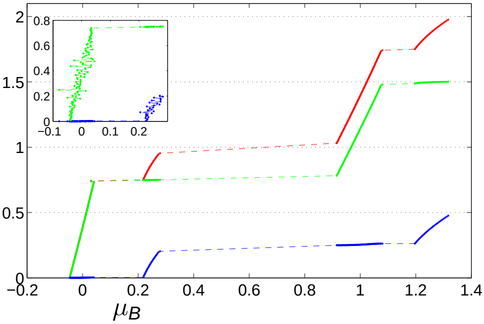
a little bit more

- lattice consits of two kinds: those with (without) fermions
- treating seperatly leads to shifted (3rd order) diagrams



is this picture allowed?

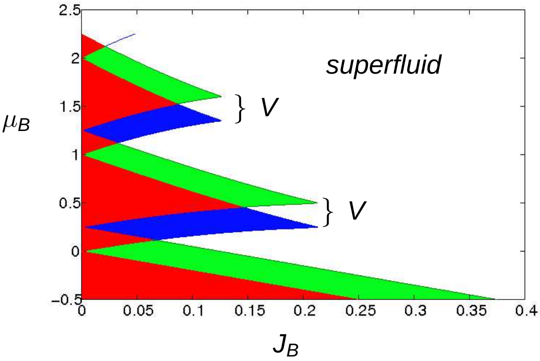
Yes it is! Consider cut along μ_B axis



Red: total mean boson density, Green: sites without fermion, Blue: sites with fermion

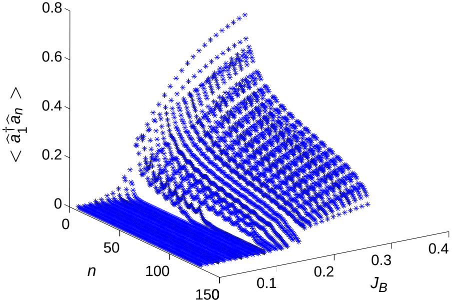
and even more

- what about shaded non incompressible regions?



What about the other regions? $\Rightarrow$ Bose Glass

Consider Correlations $\langle \hat{a}_i^\dagger \hat{a}_j \rangle$:



obvious change: exponential to algebraic

$J_F \longrightarrow \infty$: completely different

What happens in the limit $J_F \rightarrow \infty$?

First Idea:

- the fermions are totally decoupled from bosons
- since they are free, the local number operator can be replaced by density
- we expect the phase diagram of a pure BHM, shifted by $V \langle \widehat{m} \rangle = V \rho_F$

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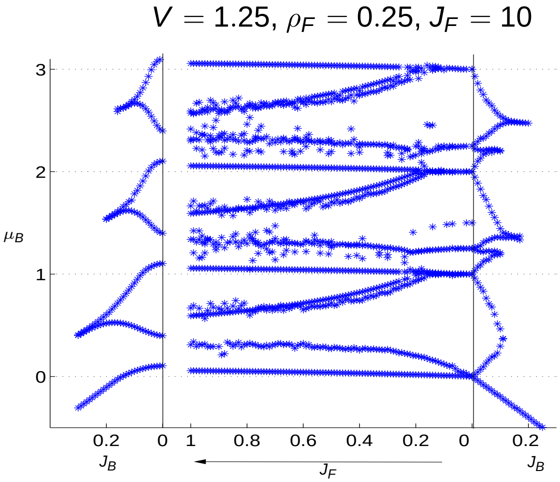
Unfortunatly (or luckily:)

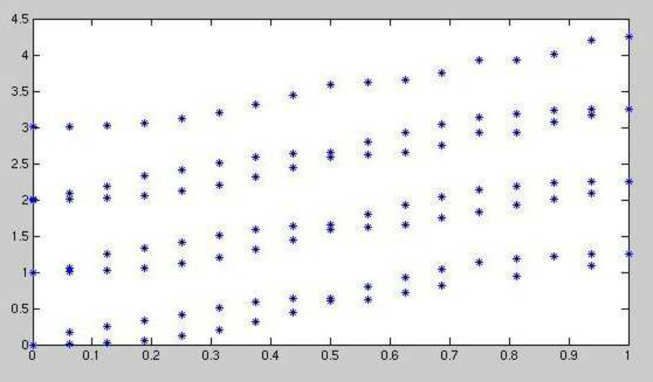
The phase diagrams looks different, but familiar!

phase diagram at $J_F \gg U, V$



gap and width at $J_B = 0$

$$V = 1.25, J_B = 0, J_F = 10$$



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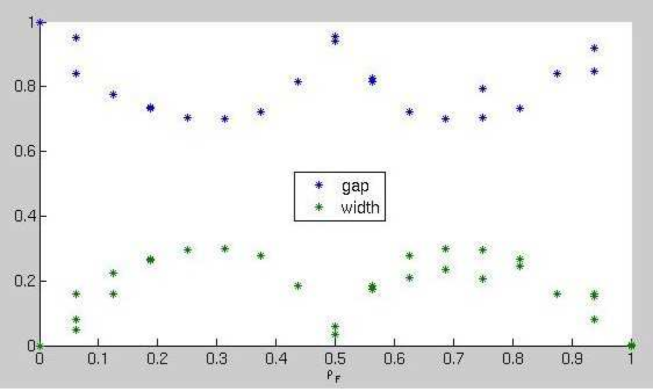

theoretical approach

Idea:

- treat fermions as bath for the bosons
- derive master equation
- therefore calculate (in interaction picture)for free fermions

$$\langle \widehat{m}_j(t)\widehat{m}_l(\tau)\rangle$$

theoretical approach

drawback

- Resulting expression:

$$\langle \widehat{m}_j(t)\widehat{m}_l(\tau)\rangle = \int_0^{2\pi\rho_F} \mathrm{d}\xi\; e^{i(\Delta D\xi - 2J_F\Delta T/\hbar\cos\xi)} \int_{2\pi\rho_F}^{2\pi} \mathrm{d}\xi'\; e^{-i(\Delta D\xi' - 2J_F\Delta T/\hbar\cos\xi')}$$

- How to calculate $\int_0^{2\pi\rho_F} \mathrm{d}\xi\; e^{i(\Delta D\xi - 2J_F\Delta T/\hbar\cos\xi)}$?
  Ideas welcome!
- alternatively give expression for $\sum_{n=-\infty}^{\infty} i^n J_n(z)\frac{x^{nB}}{x^n-\alpha}$

conclusion

- BFHM with immobile fermions can be understood by shifted BHMs
- rise up of additional, non-integer incompressible phases
- rise up of compressible phases with exponential decay

  $\Rightarrow$ Bose glass
- picture supported by correlations and density distributions
- numerics show: small fermionic hopping doesnt change a lot
- treatment of large J_F limit via master equation (?)

open questions

- for huge fermionic hopping ($J_F \gg U, V$):
  - vanishing of non-integer Mott lobes
  - Mott lobes gain a gap at $J_B = 0$
  - gap vanishes at $\rho_F = 0, 1/2, 1$
- further phases? (CDW, ...)
- hypothesis: get Bose glass boundaries in disorderd BHM by shifting the BHM properly

(first) prediction of Bose glass superfluid border ???????