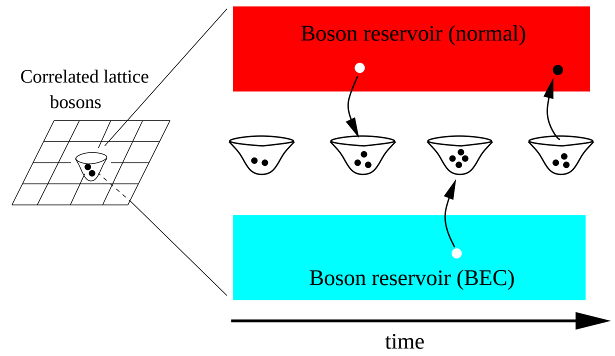
Dynamical mean-field theory for correlated bosons on a lattice in condensed and normal phases

Krzysztof Byczuk

Institute of Theoretical Physics
Department of Physics
Warsaw Univeristy



March 06th, 2009

Collaboration

Dieter Vollhardt - Augsburg University

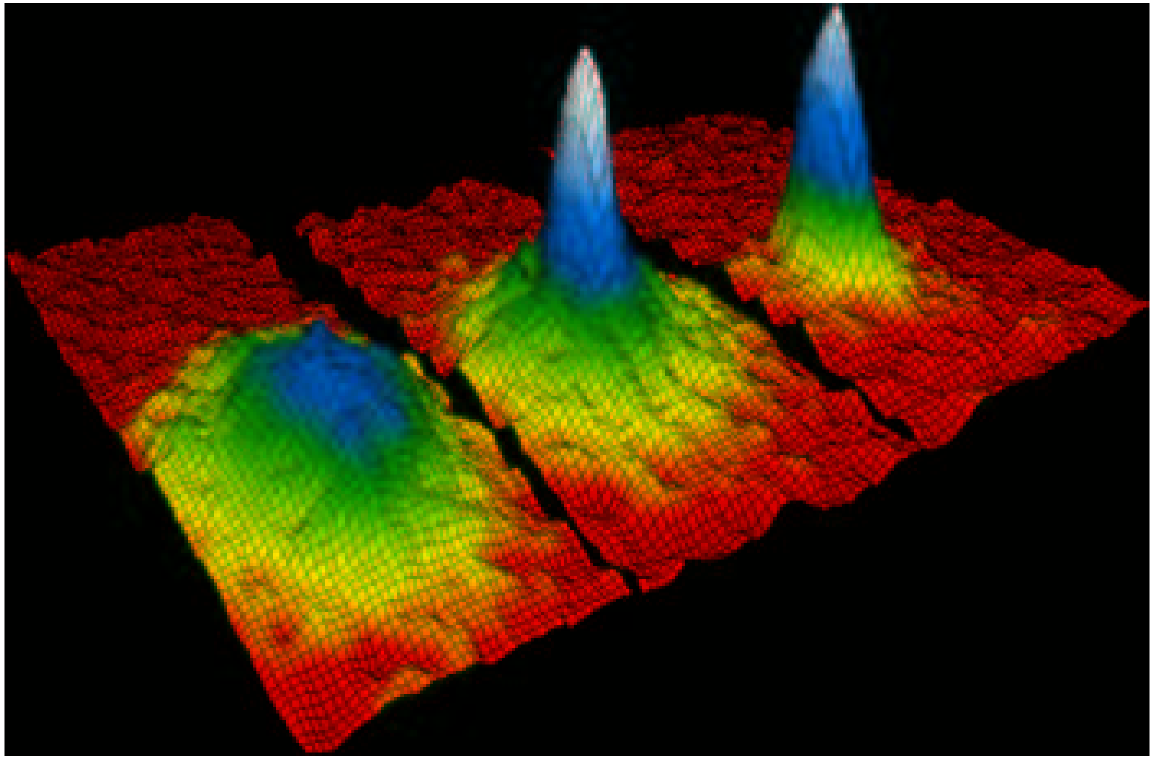
Correlated bosons on a lattice: Dynamical mean-field theory for Bose-Einstein condensed and normal phases

arXiv:0706.0839, Phys. Rev. B **77**, 235106 (2008)

Philipp Werner, Peter Anders - ETH, Zurich
Anna Kauch -Augsburg University

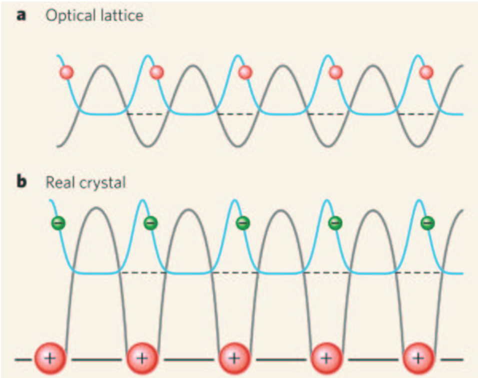
Direct Bose-Einstein condensation

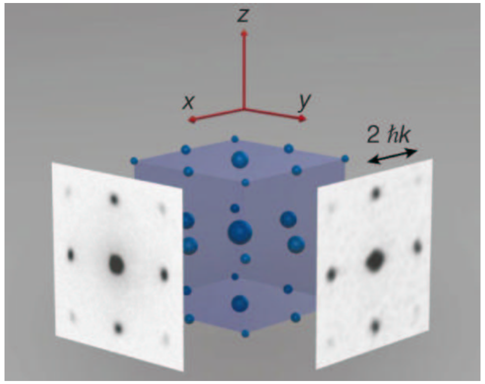
Magneto-optical traps with cold alkaline atoms with Bose statistics
(^{7}Li, ^{23}Na, ^{41}K, ^{52}Cr, ^{85}Rb, ^{87}Rb, ^{133}Cs and ^{174}Yb)

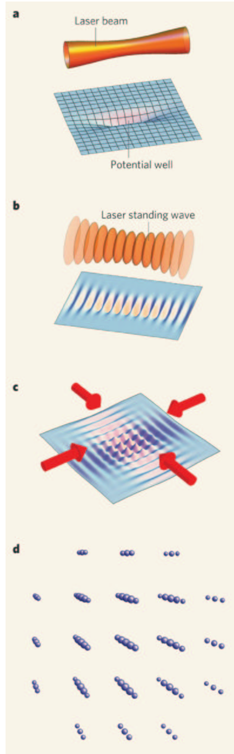


M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, 1995

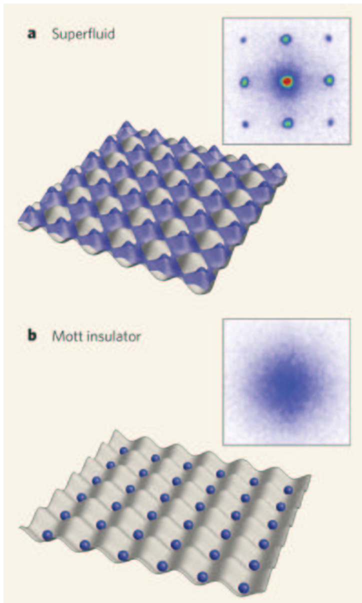
Superfluid-Mott transition - correlated lattice bosons

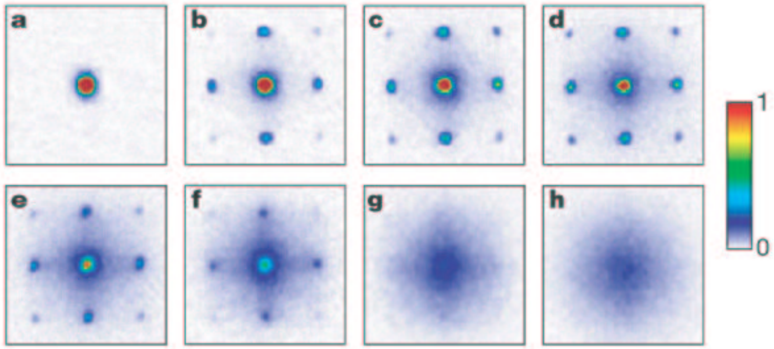






Optical lattices with cold atoms





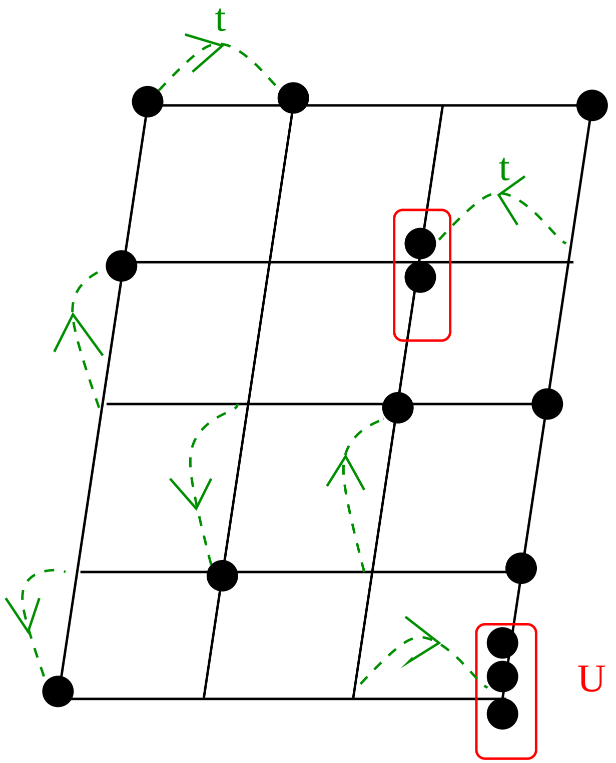
Superfluid-Mott insulator transition, Greiner, Mandel, Esslinger, Hänsch, Bloch, 2002

Correlated bosons on a lattice

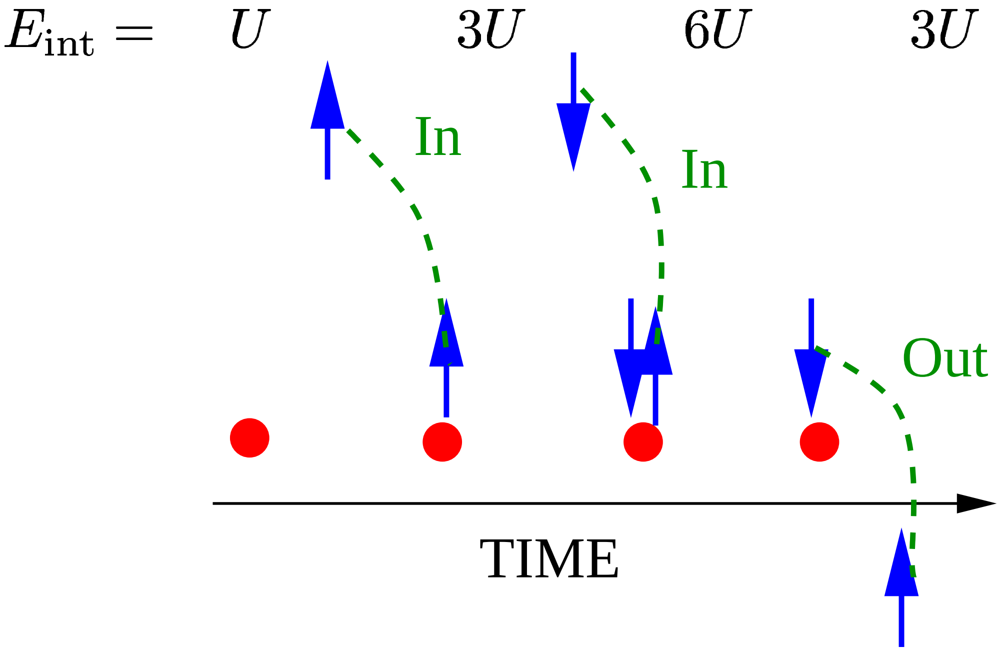
Gersch, Knollman, 1963
Fisher et al., 1989
Scalettar, Kampf, et al., 1995
Jacksch, 1998

bosonic Hubbard model

$$H = \sum_{ij} t_{ij}\, b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1)$$



local (on-site) correlations in time



$$|i,2\rangle \rightarrow |i,3\rangle \rightarrow |i,4\rangle \rightarrow |i,3\rangle$$

integer occupation of single site changes in time

Bosons on a lattice - Bose-Eisntein condensation

One-particle density matrix at $||R_i - R_j|| \to \infty$

$$\rho_{ij} = \langle b_i^\dagger b_j \rangle = \underbrace{\frac{N_c}{N_L}}_{\text{BEC part}} + \underbrace{\frac{1}{N_L} \sum_{k \neq 0} n_k e^{ik(R_i - R_j)}}_{\text{normal part}} \underbrace{\longrightarrow}_{||R_i - R_j|| \to \infty} \frac{N_c}{N_L} = n_c$$

- BEC part – constant
- normal part – vanishes

The two contributions to the density matrix behave differently

Standard approximations

- Bose-Einstein condensation treated by Bogoliubov method $b_i = \langle b_i \rangle + \tilde{b}_i$ where $\langle b_i \rangle \equiv \phi_i \in C$ classical variable (Bogoliubov 1947)

- Weak coupling - mean-field (expansion) in U, valid for small U, average on-site density, local correlations in time neglected (Ooste, Stoof, et al., 2000)

- Strong coupling - mean-field (expansion) in t, valid for small t (Freericks, Monien, 1994; Kampf, Scalettar, 1995)

Bose-Einstein condensate – Mott insulator transition

$$U \sim t$$

intermediate coupling problem

Comprehensive mean-field theory needed

Comprehensive mean-field theory

- valid for all parameters values t, U, n, T,..
- thermodynamically consistent
- conserving
- small (control) parameter $1/d$

$d \to \infty \Rightarrow$ Dynamical mean-field theory for lattice bosons (B-DMFT)

Problem: How to rescale the kinetic energy with d?

Quantum lattice bosons in $d \to \infty$ limit

W. Metzner and D. Vollhardt 1989 - rescaling of hopping amplitudes for fermions

$$t_{ij} = \frac{t^*_{ij}}{(2d)^{\frac{||R_i - R_j||}{2}}} \qquad \text{for NN } i,j \qquad t = \frac{t^*}{\sqrt{Z}}, \quad Z = 2d$$

Not sufficient for bosons because of BEC:

$$\text{Normal bosons}: \quad \langle H_{kin} \rangle = -\underbrace{t}_{\frac{1}{\sqrt{Z}}} \sum_i \underbrace{\sum_{j(NN\ i)}}_{Z} \underbrace{\langle b_i^\dagger b_j \rangle}_{\frac{1}{\sqrt{Z}}} \neq \infty, 0 \quad \Rightarrow \quad \text{rescaling} \quad t = \frac{t^*}{\sqrt{Z}}$$

$$\text{BEC bosons}: \quad \langle H_{kin} \rangle = -\underbrace{t}_{\frac{1}{Z}} \sum_i \underbrace{\sum_{j(NN\ i)}}_{Z} \underbrace{\langle b_i^\dagger \rangle \langle b_j \rangle}_{Z-\text{independent}} \neq \infty, 0 \quad \Rightarrow \quad \text{rescaling} \quad t = \frac{t^*}{Z}$$

No way to construct comprehensive mean-field theory
in the bare Hamiltonian operator formalism

BEC and normal bosons on the lattice in $d \to \infty$ limit

1. Rescaling is made inside a thermodynamical potential (action, Lagrangian) but not at the level of the Hamiltonian operator
   - normal parts: $t_{ij} = \frac{t^*_{ij}}{(2d)^{\frac{||R_i - R_j||}{2}}}$ - fractional rescaling
   - BEC parts: $t_{ij} = \frac{t^*_{ij}}{(2d)^{||R_i - R_j||}}$ - integer rescaling
2. Limit $d \to \infty$ taken afterwards in this effective potential

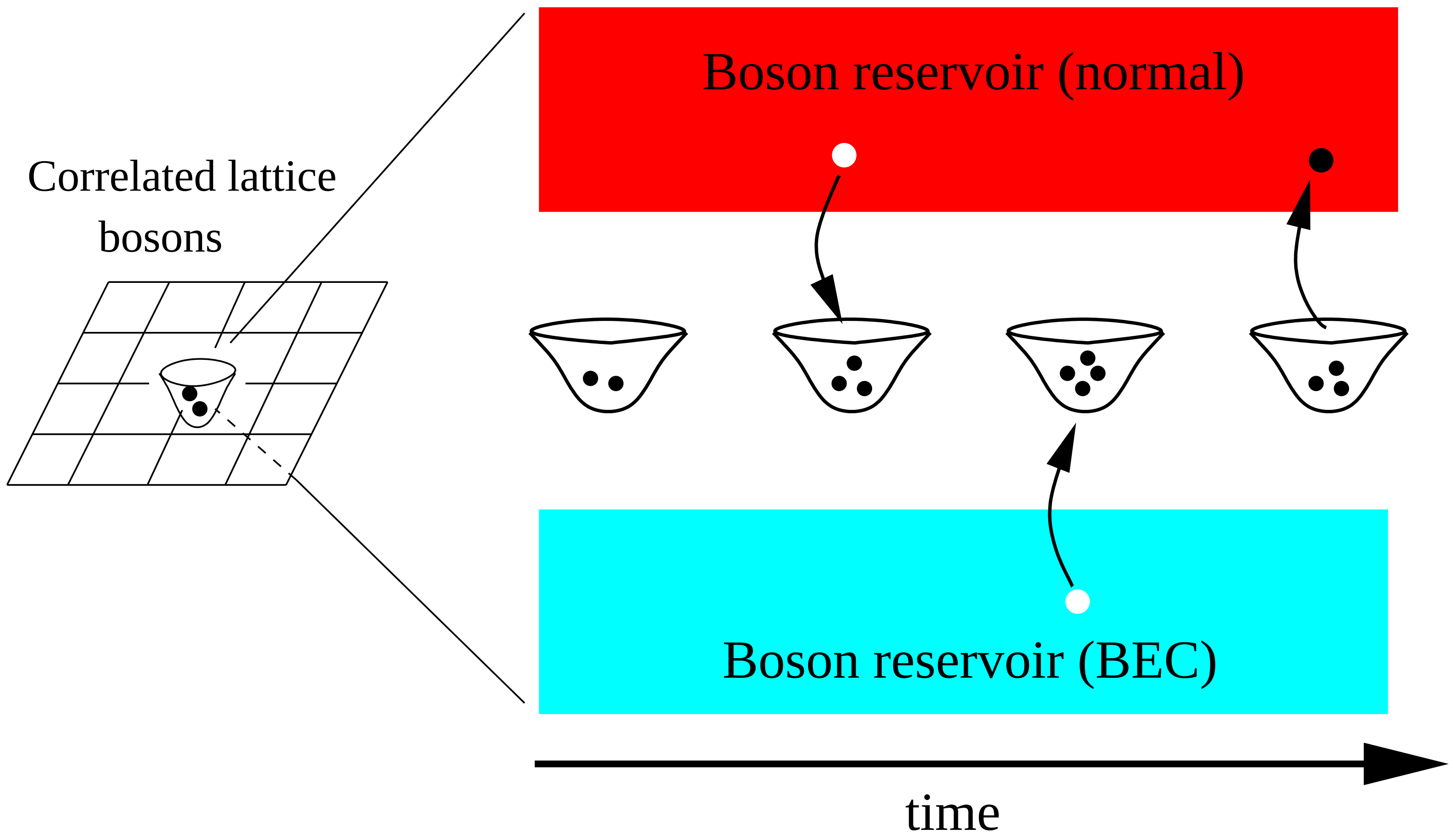
Only this procedure gives consistent derivation of B-DMFT equations as exact ones in $d \to \infty$ limit for boson models with local interactions

Normal and condensed bosons are on equal footing already in $d \to \infty$ limit

KB, Vollhardt, Phys. Rev. B **77**, 235106 (2008): systematic linked cluster expansion with correct rescaling of different terms, $d \to \infty$ limit, gathering all non-vanishing terms into exponent

Bosonic-Dynamical Mean-Field Theory (B-DMFT)

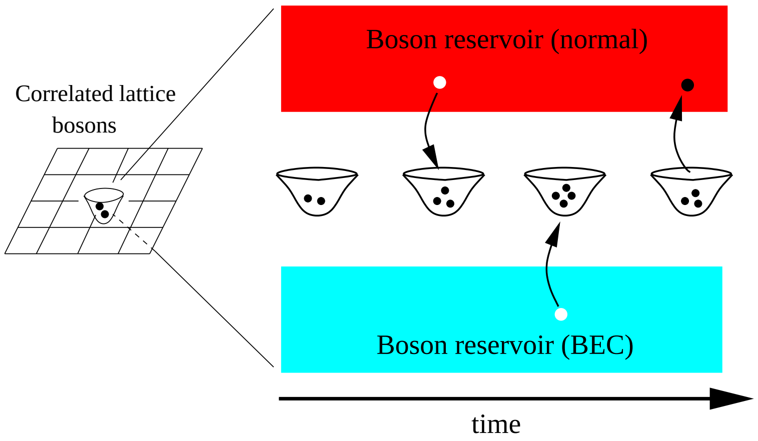
- Exact mapping of the lattice bosons in infinite dimension onto a single site
- Single site coupled to two reservoirs: normal bosons and bosons in the condensate
- Reservoirs properties are determined self-consistently, local correlations kept



B-DMFT application to bosonic Hubbard model

(i) Lattice self-consistency equation (exact in $d \to \infty$)

$$\hat{G}(i\omega_n) = \int d\epsilon N_0(\epsilon) \left[\begin{pmatrix} i\omega_n + \mu - \epsilon & 0 \\ 0 & -i\omega_n + \mu - \epsilon \end{pmatrix}^{-1} - \hat{\Sigma}(i_{\omega_n}) \right]^{-1}$$



(ii) Local impurity $\hat{G}(\tau) = \int D[b^*, b]\ \bar{b}(\tau)\bar{b}^*(0)\ e^{-S_{loc}}$

$$S_{loc} = -\int_0^\beta \int_0^\beta d\tau d\tau' \bar{b}^\dagger(\tau)\ \hat{\mathcal{G}}^{-1}(\tau - \tau')\ \bar{b}(\tau) +$$

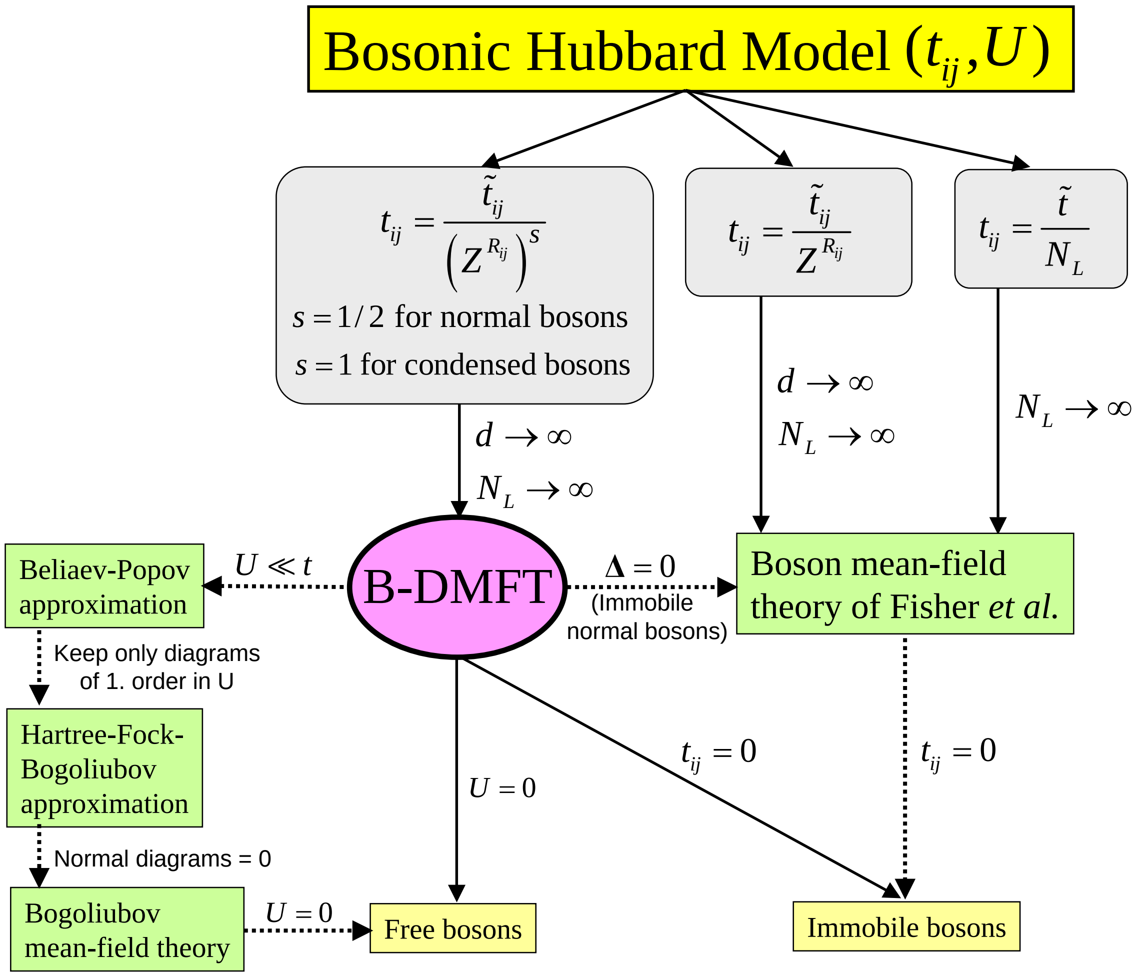
$$\kappa \int_0^\beta d\tau \bar{\phi}^\dagger(\tau)\bar{b}(\tau) + \frac{U}{2} \int_0^\beta n(\tau)(n(\tau) - 1)$$

$$\hat{\mathcal{G}}^{-1}(i_{\omega_n}) = \hat{G}^{-1}(i_{\omega_n}) + \hat{\Sigma}(i_{\omega_n}) = \begin{pmatrix} i\omega_n + \mu & 0 \\ 0 & -i\omega_n + \mu \end{pmatrix} - \hat{\Delta}(i\omega_n)$$

(iii) Condensate wave function

$\bar{\phi}(\tau) = \int D[b^*, b]\ \bar{b}(\tau)\ e^{-S_{loc}}$,   A.Kauch: proof that $\bar{\phi}(\tau) = \text{const}$

B-DMFT in well-known limits



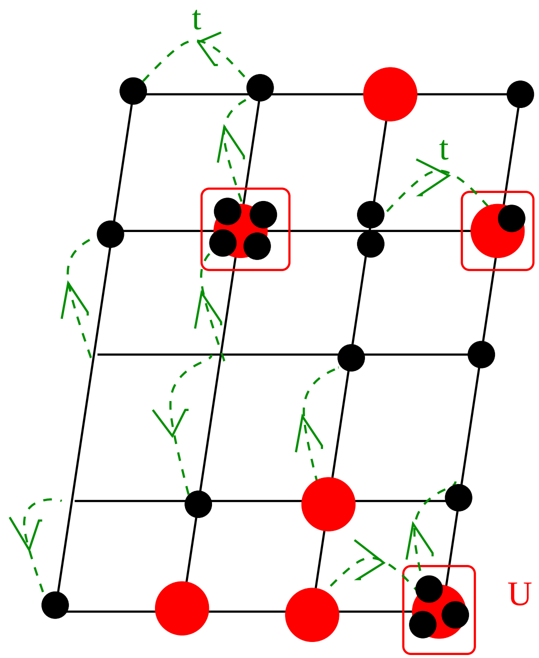
Application I: bosonic Falicov-Kimball model

Binary mixture of itinerant (b) and localized (f) bosons on the lattice

$$H = \sum_{ij} t_{ij}\, b_i^\dagger b_j + \epsilon_f \sum_i f_i^\dagger f_i + U_{bf} \sum_i n_{bi} n_{fi} + U_{ff} \sum_i n_{fi} n_{fi}$$

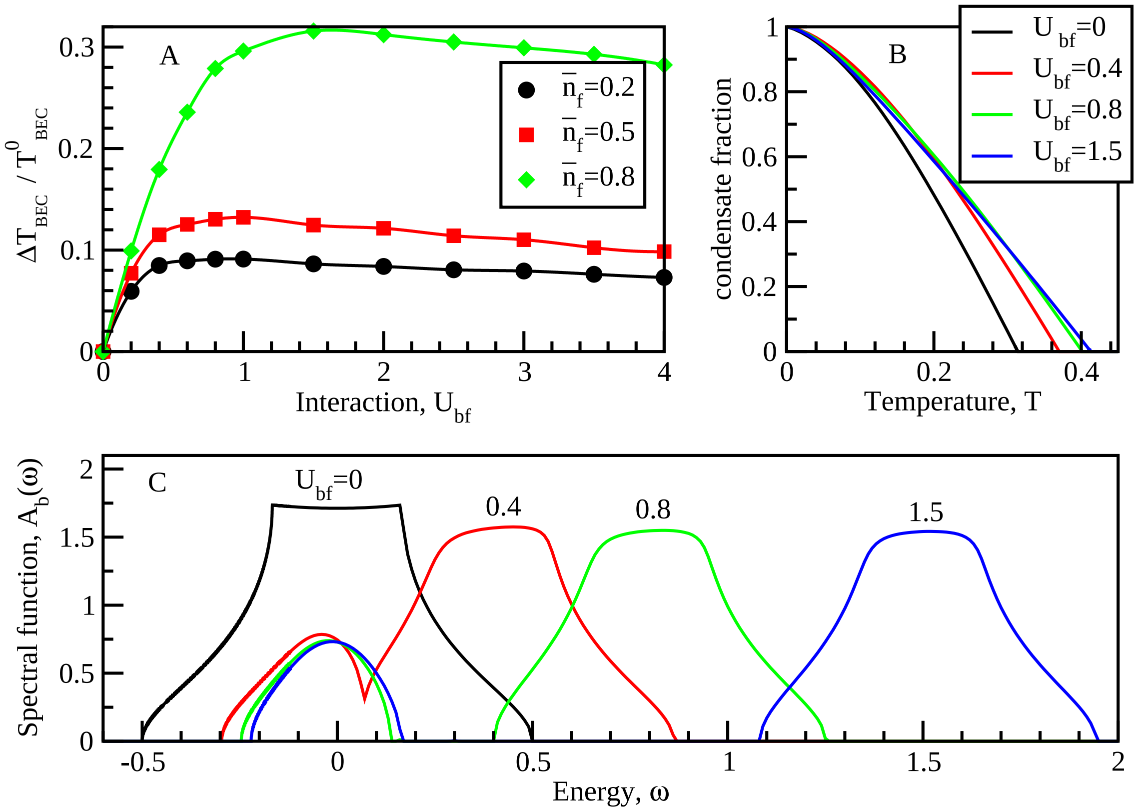
Local conservation law $[n_{fi}, H] = 0$ hence $n_{fi} = 0, 1, 2, \ldots$ classical variable

B-DMFT: local action Gaussian and analytically integrable



Enhancement of T_{BEC} due to interaction

Hard-core f-bosons $U_{ff} = \infty$; $n_f = 0, 1$; $0 \le \bar{n}_f \le 1$; $d = 3$ - SC lattice



KB, Vollhardt, PRB (2008)

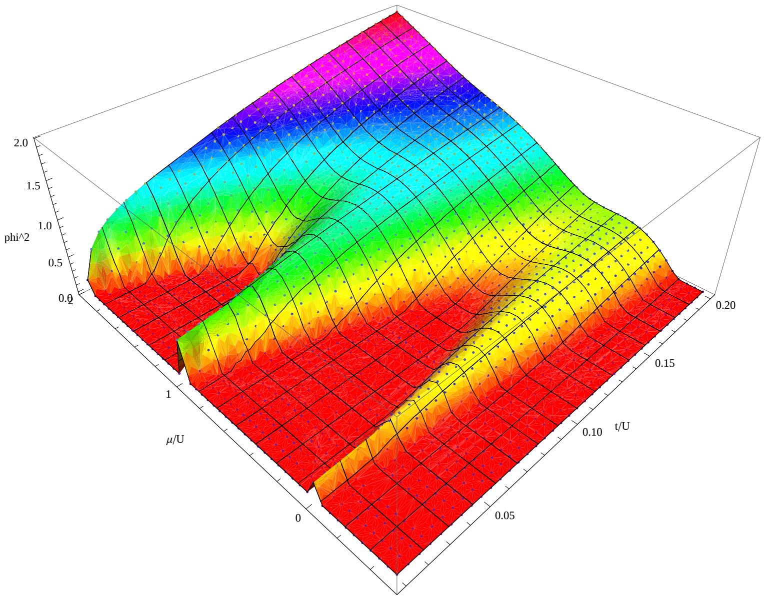
$$A_b(\omega) = -\mathrm{Im} G_b(\omega)/\pi$$

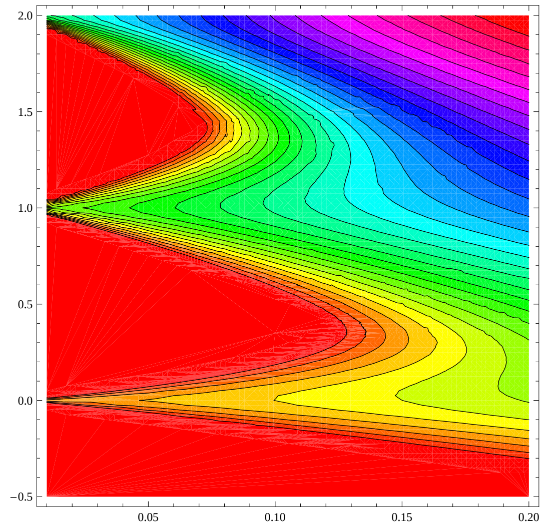
$$\bar{n}_b = \bar{n}_b^{BEC} + \int d\omega \, \frac{A_b(\omega+\mu_b)}{e^{\omega/T}-1}$$

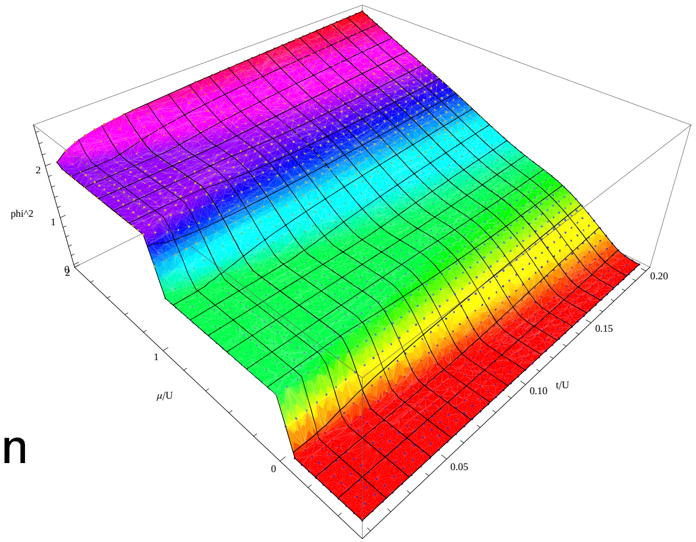
Normal part decreases when U increases for constant μ_b and T

Application II: bosonic Hubbard model CT-QMC

Philipp Werner, Peter Anders: developed continous time Monte Carlo method for local (impurity) bosonic problem with B-DMFT self-consistency conditions





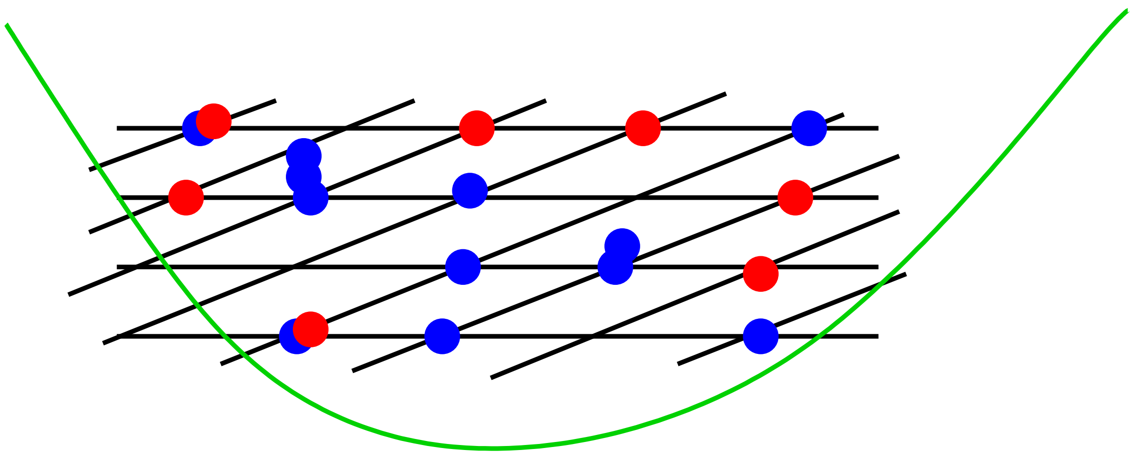


Exact result for SF-Mott Insulator transition

Bethe DOS, $W = 4$, $\beta = 4$

Application III:
Bose-Fermi mixture (^{87}Rb-^{40}K) on a lattice in a trap

$$H = \sum_{ij} t^b_{ij} b^\dagger_i b_j + \sum_i \epsilon^b_i n^b_i + \frac{U_b}{2} \sum n^b_i (n^b_i - 1) + \sum_{ij} t^f_{ij} f^\dagger_i f_j + \sum_i \epsilon^f_i n^f_i + U_{bf} \sum_i n^b_i n^f_i$$



DMFT for bose-fermi mixtures

BF-DMFT equations:

$$S_{i_0}^{\mathrm{b}} = \int_0^\beta d\tau \mathbf{b}_{i_0}^\dagger(\tau) \left(\partial_\tau \sigma_{\mathbf{3}} - (\mu_b - \epsilon_{i_0}^b)\mathbf{1}\right) \mathbf{b}_{i_0}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' \mathbf{b}_{i_0}^\dagger(\tau) \mathbf{\Delta}_{i_0}^b(\tau - \tau') \mathbf{b}_{i_0}(\tau')$$

$$+ \frac{U_b}{\mathbf{2}} \int_0^\beta n_{i_0}^b(\tau)(n_{i_0}^b(\tau) - 1) + \int_0^\beta d\tau \sum_{j \neq i_0} t_{i_0 j}^b \mathbf{b}_{i_0}^\dagger(\tau) \mathbf{\Phi}_j(\tau)$$

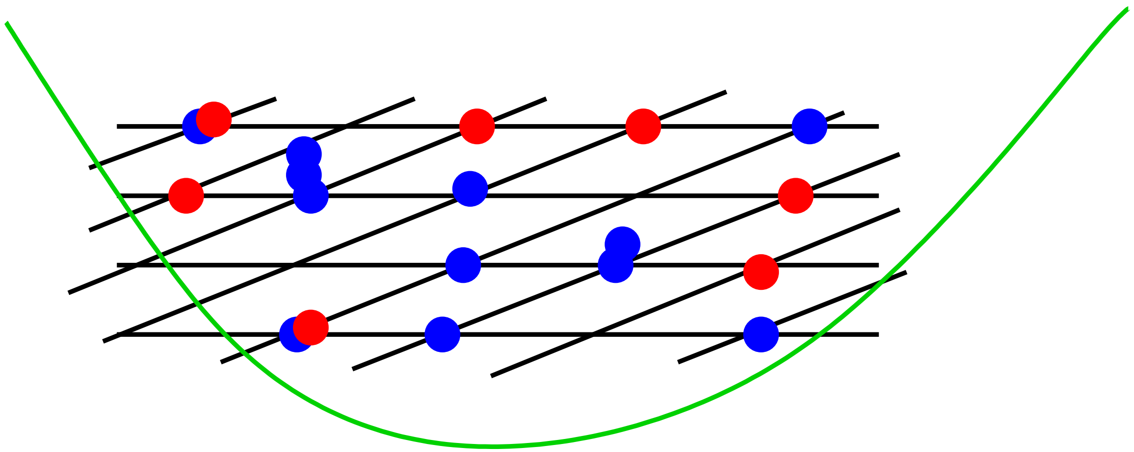
$$S_{i_0}^{\mathrm{f}} = \int_0^\beta d\tau f_{i_0}^*(\tau) \left(\partial_\tau - \mu_f + \epsilon_{i_0}^f\right) f_{i_0}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' f_{i_0}^*(\tau) \Delta_{i_0}^f(\tau - \tau') f_{i_0}(\tau')$$

$$S_{i_0}^{\mathrm{bf}} = U_{bf} \int_0^\beta d\tau n_{i_0}^b(\tau) n_{i_0}^f(\tau)$$

Lattice self-consistency (Dyson) equations

$$\mathbf{G}^b_{ij}(i\nu_n) = \left[(i\nu_n\sigma_3 + \mu_b\mathbf{1} - \mathbf{\Sigma}^b_i(i\nu_n))\delta_{ij} - t^b_{ij}\mathbf{1}\right]^{-1}$$

$$G^f_{ij}(i\omega_n) = \left[(i\omega_n + \mu_f - \Sigma^f_i(i\omega_n))\delta_{ij} - t^f_{ij}\right]^{-1}$$



Effective interaction between bosons

Integrating out fermions: effective bosonic action

$$\tilde{S}^b_{i_0} \approx S^b_{i_0} + \frac{U_{bf}}{\sqrt{\beta}} \sum_n \mathcal{G}^f_{i_0}(\omega_n) n^b_{i_0}(\nu_m = 0) - \frac{U^2_{bf}}{2} \sum_n n^b_{i_0}(\nu_n) \pi^f_{i_0}(\nu_n) n^b_{i_0}(-\nu_n)$$

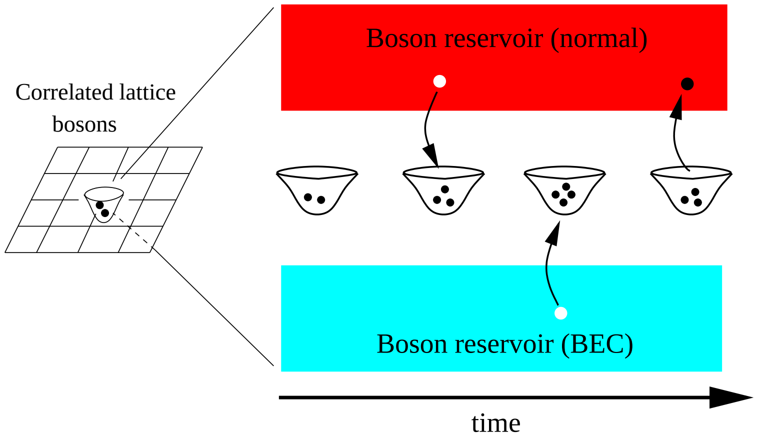
$$\pi^f_{i_0}(\nu_n) \equiv -\frac{1}{\beta} \sum_m \mathcal{G}^f_{i_0}(\omega_m) \mathcal{G}^f_{i_0}(\omega_m + \nu_n)$$

with renormalized boson-boson interaction

$$U_b^{\text{eff}} = U_b - U^2_{bf} N^f_{i_0}(\mu)$$

system unstable when $U_b = U^2_{bf} N^f_{i_0}(\mu)$.

Summary and Outlook



- Bosonic Dynamical Mean-Field Theory
  - comprehensive mean-field theory
  - conserving and thermodynamically consistent
  - exact in $d \to \infty$ limit due to new rescaling
- B-DMFT equations and CT-QMC solution for bosonic Hubbard model
- B-DMFT solution for bosonic Falicov-Kimball model
  - Enhancement of T_{BEC} due to correlations
  - Mixture of ^{87}Rb (f-bosons) and ^{7}Li (b-bosons) may have larger T_{BEC} on optical lattices
- Spinor bosons, bose-fermi mixture within B-DMFT or density like LRO easy to include within B-DMFT
- More bosonic impurity solvers wanted!