Dynamical mean-field theory for lattice bosons

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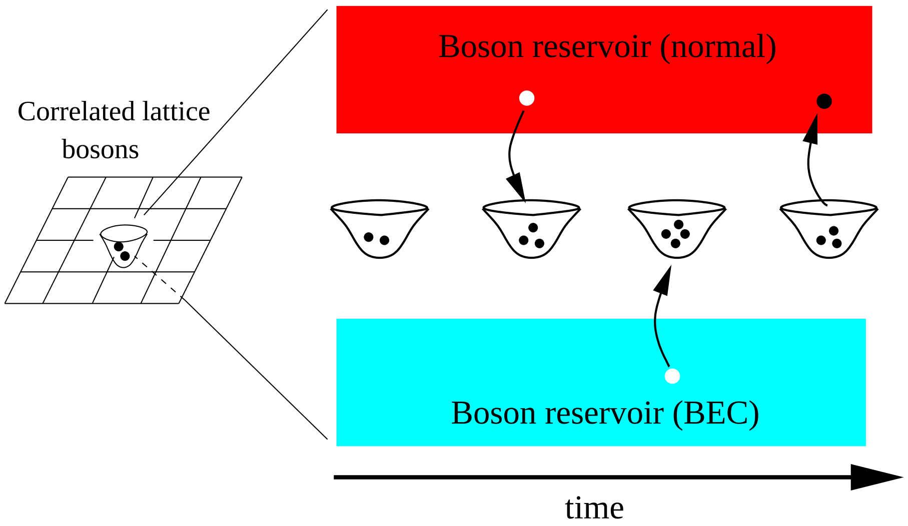
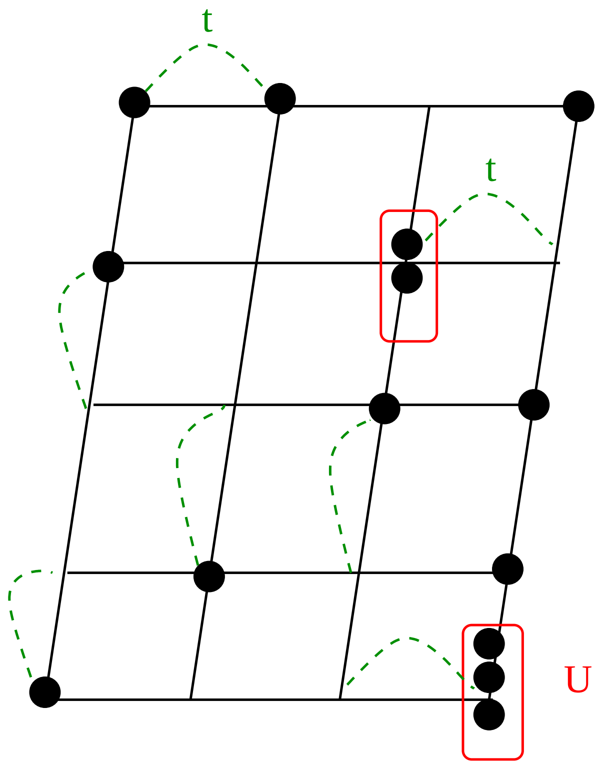


Correlated bosons on optical lattices

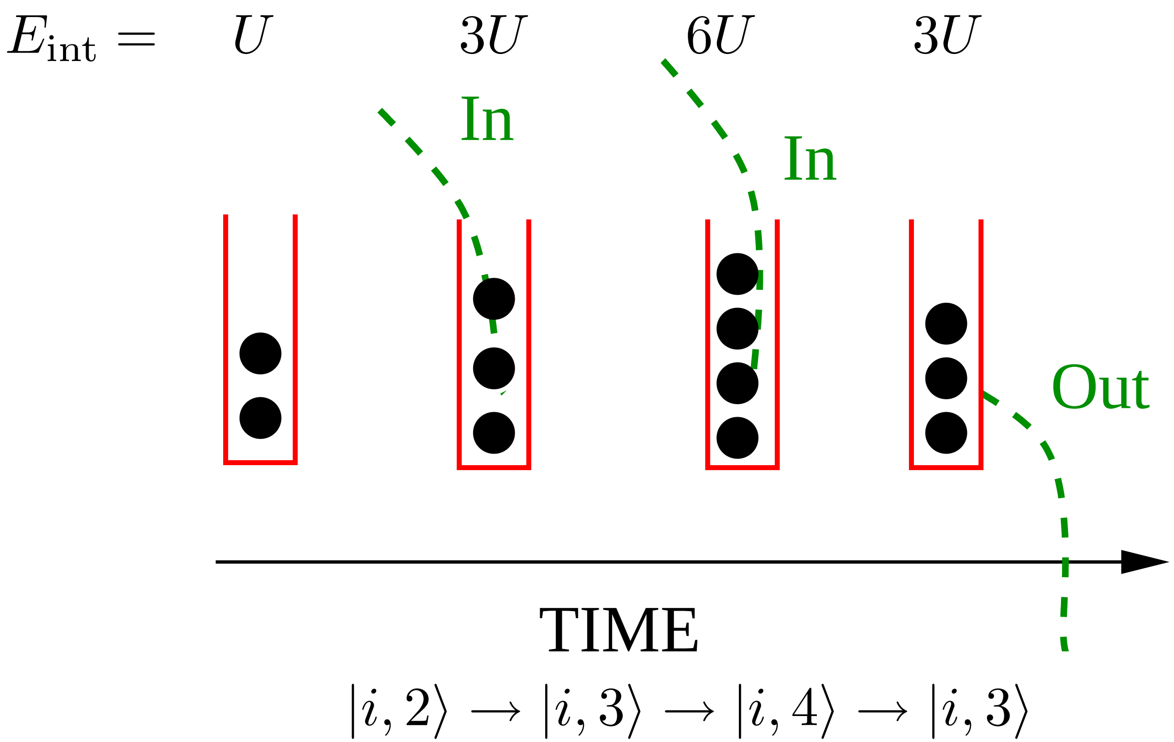
Gersch, Knollman, 1963
Fisher et al., 1989
Scalettar, Kampf, et al., 1995
Jacksch, 1998

Bose - 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



integer occupation of single site changes in time

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

Like DMFT for fermions: exact and non-trivial in $d \to \infty$ limit

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

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

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

Not sufficient for bosons because of BEC:

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

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

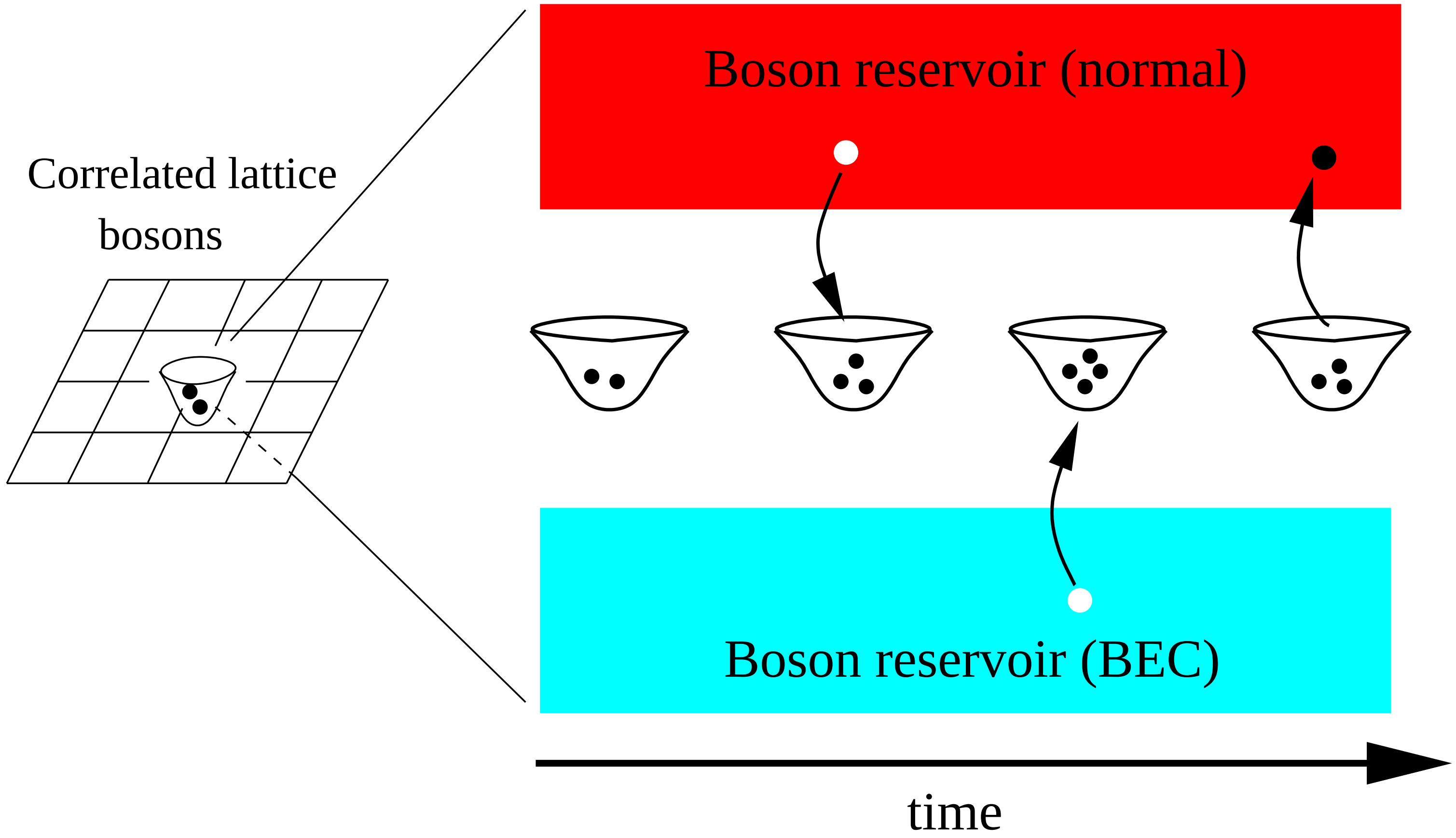
   - normal parts: $t_{ij} = \frac{t^*_{ij}}{(2d)^{\frac{||R_i - R_j||}{2}}}$ - quantum rescaling
   - BEC parts: $t_{ij} = \frac{t^*_{ij}}{(2d)^{||R_i - R_j||}}$ - classical rescaling

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

Bosonic-Dynamical Mean-Field Theory

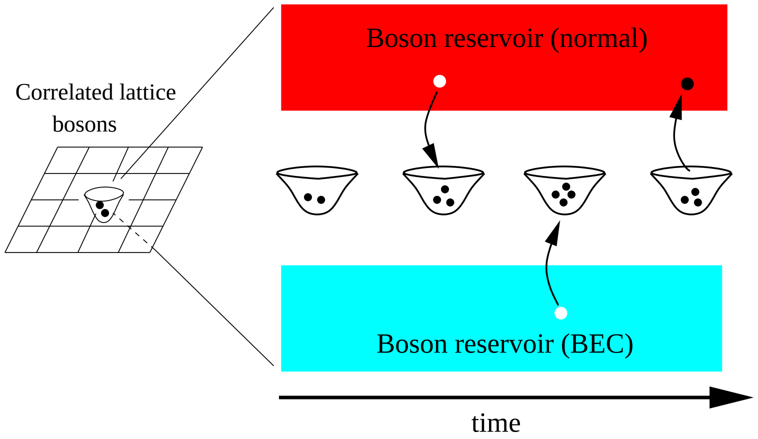
- Exact mapping of the lattice bosons in infinite dimension onto a single site
- Single site coupled to two reservoirs: normal bosons and bosons in the condensate
- Reservoirs properties are determined self-consistently, local correlations kept



Application for Bose-Hubbard model

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

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



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

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

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

(iii) Generalized Gross-Pitaevskii eq. (exact in $d \to \infty$)

$$\partial_\tau \bar{\phi}(\tau) - \int_0^\beta d\tau' \widehat{\Delta}(\tau - \tau')\bar{\phi}(\tau') + \kappa\bar{\phi}(\tau) + U|\bar{\phi}(\tau)|^2\bar{\phi}(\tau) = \mu\bar{\phi}(\tau)$$

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

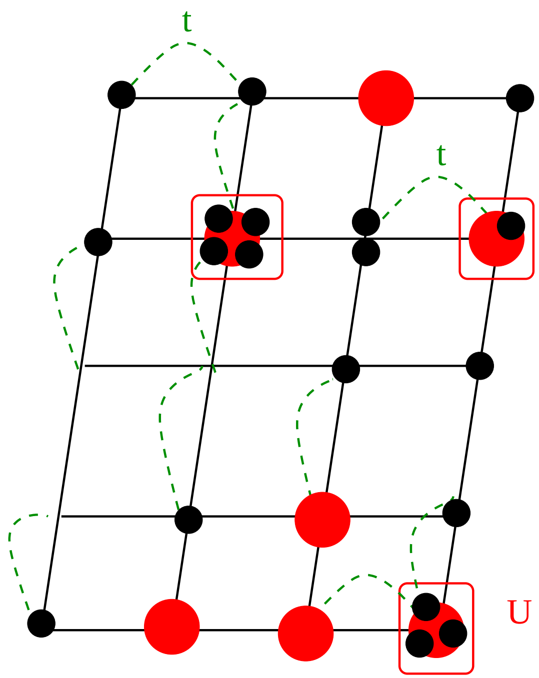
Application for Bose-Falicov-Kimball model

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

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

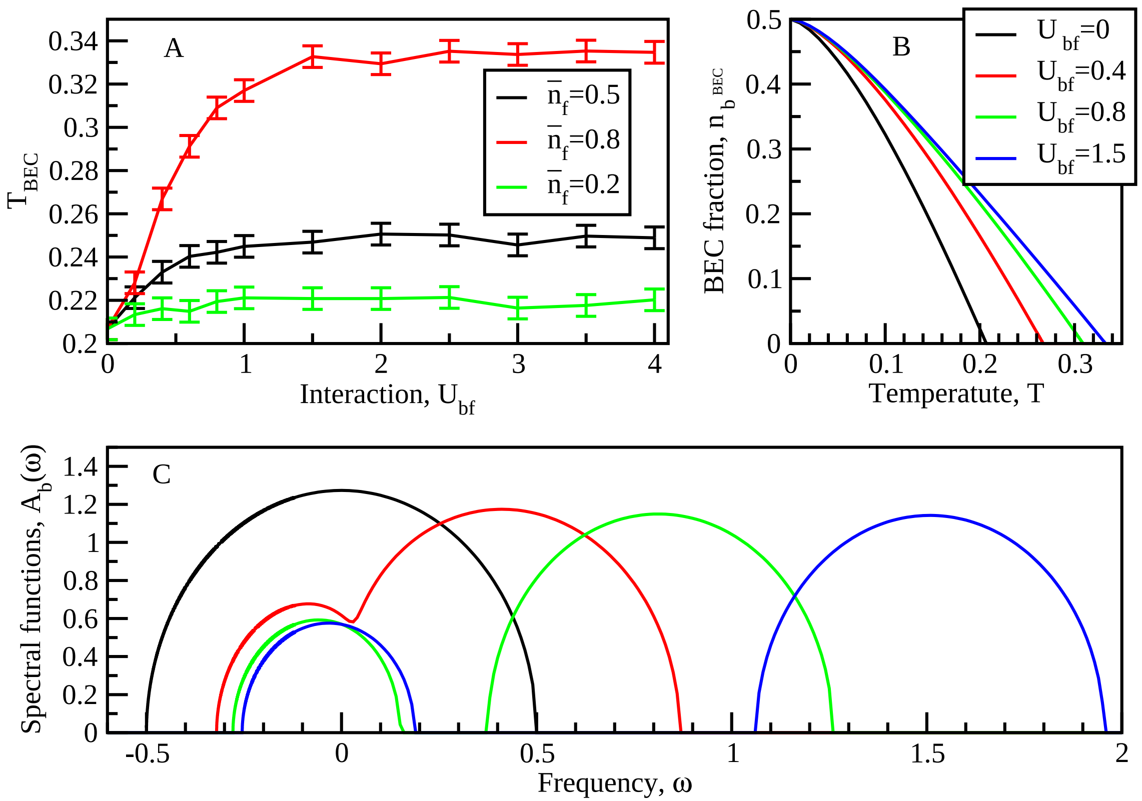
Local conservation law $[n_{fi}, H] = 0$ hence $n_{fi} = 0, 1, 2, ...$ classical variable

B-DMFT: local action Gaussian and analytically integrable



Enhancement of T_{BEC} due to interaction

Hard-core f-bosons $U_{ff} = \infty$; $n_f = 0, 1$; $0 \leq \bar{n}_f \leq 1$



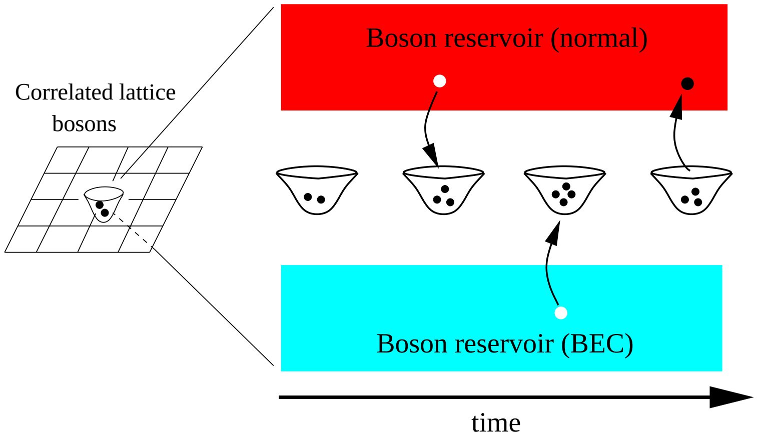
$$A_b(\omega) = -\mathrm{Im}G_b(\omega)/\pi$$

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

Normal part decreases when U increases for constant μ_b and T

Summary and Outlook

- Formulated Bosonic Dynamical Mean-Field Theory (B-DMFT)
  - comprehensive mean-field theory
  - conserving and thermodynamically consistent
  - exact in $d \to \infty$ limit due to new rescaling



- B-DMFT equations for Bose-Hubbard model

- B-DMFT solution for Bose-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