Dynamical mean-field theory for correlated lattice bosons in Bose-Einstein and normal phases

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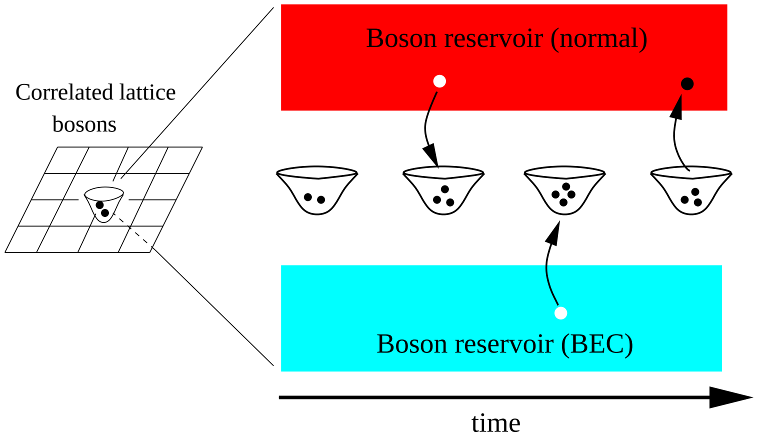
Main results

- New comprehensive dynamical mean-field theory for correlated, lattice bosons in normal and condensate phases, exact in $d \to \infty$



- Correlation might enhance BEC fraction and transition temperature

Collaboration

Dieter Vollhardt - Augsburg University

Preprint

Correlated bosons on a lattice: Dynamical mean-field theory for Bose-Einstein condensed and normal phases - arXiv:0706.0839

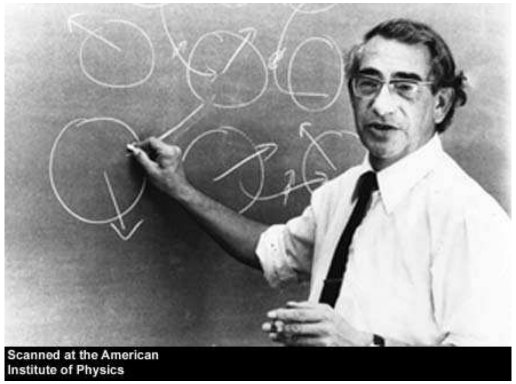
Plan of talk

- Dynamical mean-field theory (DMFT) for correlated fermions
- Formulation of dynamical mean-field theory for bosons (B-DMFT)
- Bosonic Hubbard model within B-DMFT
- Falicov-Kimball model within B-DMFT
  - Enhancement of BEC transition temperature due to correlations
- Summary and outlook

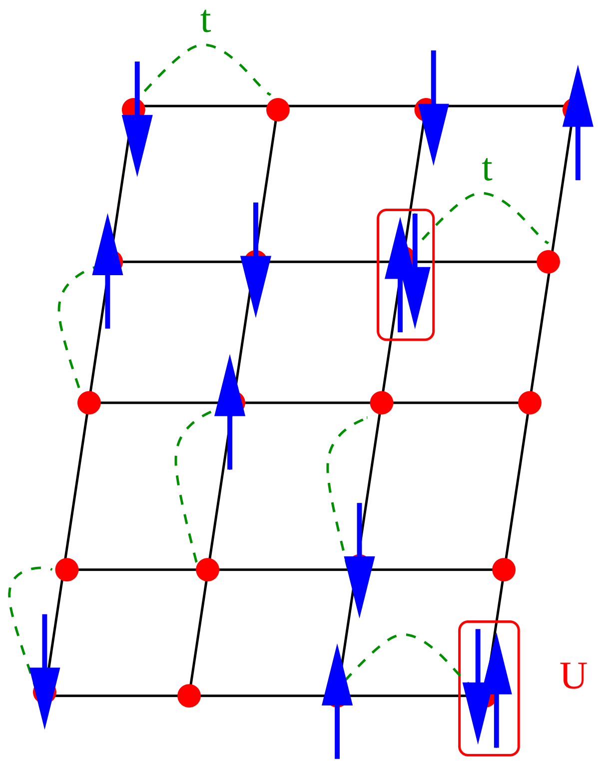
FERMIONS

Correlated lattice fermions

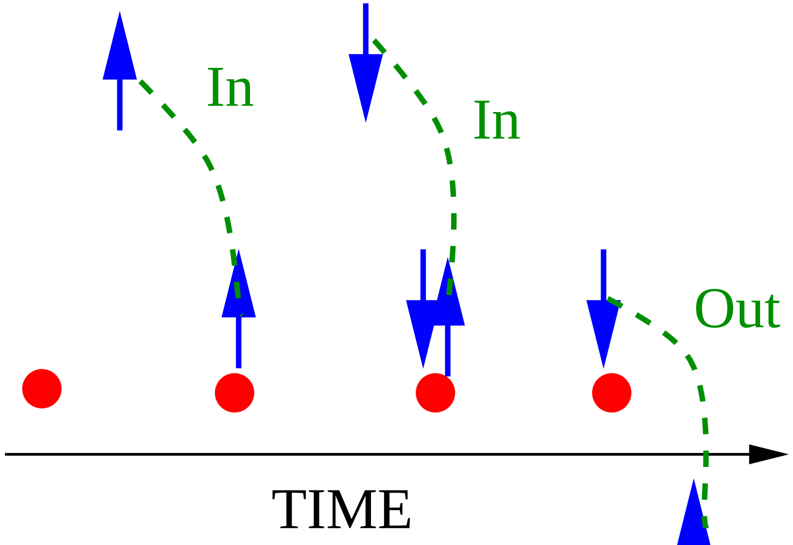
$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



fermionic Hubbard model, 1963



Local Hubbard physics



$$|i,0\rangle \rightarrow |i,\uparrow\rangle \rightarrow |i,2\rangle \rightarrow |i,\downarrow\rangle$$

The Holy Grail for correlated electrons (fermions)

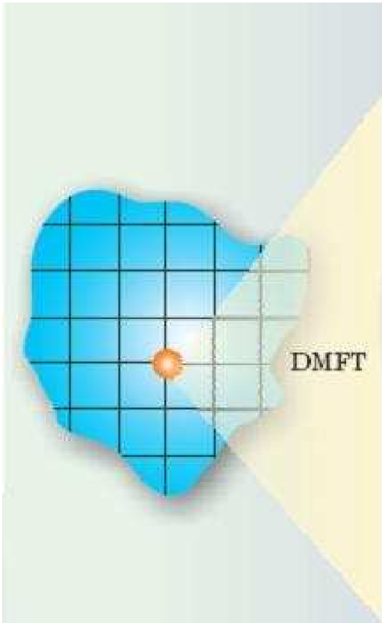
Fact: Hubbard model is not solved for arbitrary cases

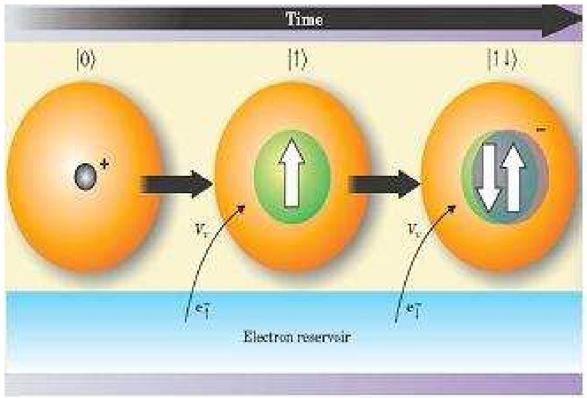
Find the best comprehensive approximation

- valid for all values of parameters t, U, $n = N_e/N_L$, T, all thermodynamic phases
- thermodynamically consistent
- conserving
- possessing a small expansion (control) parameter and exact in some limit
- flexible to be applied to different systems and material specific calculations

DMFT for lattice fermions

Replace (map) full many-body lattice problem by a single-site coupled to dynamical reservoir and solve such problem self-consistently





All local dynamical correlations included exactly

Space correlations neglected - mean-field approximation

DMFT - equations full glory

Local Green function

$$G_\sigma(\tau) = -\langle T_\tau c_\sigma(\tau) c_\sigma^*(0)\rangle_{S_{loc}}$$

where

$$S_{loc} = -\sum_\sigma \int d\tau d\tau' c_\sigma^*(\tau)\mathcal{G}_\sigma^{-1}(\tau-\tau')c_\sigma(\tau') + U\int d\tau n_\uparrow(\tau)n_\downarrow(\tau)$$

Weiss (mean-field) function and self-energy

$$\mathcal{G}_\sigma^{-1}(\omega_n) = G_\sigma^{-1}(\omega_n) + \Sigma_\sigma(\omega_n)$$

Local Green function and lattice system self-consistency

$$G_\sigma(i\omega_n) = \sum_{\mathbf{k}} G_\sigma(\mathbf{k},\omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\omega_n)} = G_\sigma^0(i\omega + \mu - \Sigma_\sigma(\omega_n))$$

DMFT - exact in the infinite dimension (coordination)

Non-trivial (asymptotic) theory is well defined such that the energy density is generically finite and non-zero

$$\frac{1}{N_L}E_{kin} = \frac{1}{N_L}\sum_{ij\sigma} t_{ij}\langle c^\dagger_{i\sigma} c_{j\sigma}\rangle = \frac{1}{N_L}\sum_{i\sigma} \underbrace{\sum_{j(i)}}_{O(d^{||\mathbf{R}_i-\mathbf{R}_j||})} t_{ij} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} G_{ij\sigma}(\omega) \sim O(1)$$

Fact, since G_{ij} is probability amplitude for hopping,

$$G_{ij} \sim O(d^{-\frac{||\mathbf{R}_i-\mathbf{R}_j||}{2}})$$

with rescaling

$$t_{ij} \to \frac{t^*_{ij}}{\sqrt{d^{||\mathbf{R}_i-\mathbf{R}_j||}}}$$

sum $\sum_{j(i)}$ is compensated and energy is finite (Metzner, Vollhardt, 1989)

$d \to \infty$ limit – Feynman diagrams simplification

One proves, term by term, that skeleton expansion for the self-energy $\Sigma_{ij}[G]$ has only local contributions

$$\Sigma_{ij\sigma}(\omega_n) \to_{d\to\infty} \Sigma_{ii\sigma}(\omega_n)\delta_{ij}$$

Fourier transform is $\mathbf{k}$-independent

$$\Sigma_\sigma(\mathbf{k},\omega_n) \to_{d\to\infty} \Sigma_\sigma(\omega_n)$$

DMFT is an exact theory in infinite dimension (coordination number) and small control parameter is $1/d$ ($1/z$)

(Metzner, Vollhardt, 1989)

DMFT – flexibility; LDA+DMFT

Multi-band systems (Anisimov et al. 97; ... Nekrasov et al. 00, ...)

$$H = H_{LDA} + H_{int} - H_{LDA}^{U} = H_{LDA}^{0} + H_{int}$$

direct and exchange interaction

$$H_{int} = \frac{1}{2} \sum_{i=i_d, l=l_d} \sum_{m\sigma, m'\sigma'} U_{mm'}^{\sigma\sigma'} \, n_{ilm\sigma} n_{ilm'\sigma'}$$

$$-\frac{1}{2} \sum_{i=i_d, l=l_d} \sum_{m\sigma, m'} J_{mm'} \, c_{ilm\sigma}^{\dagger} c_{ilm'-\sigma}^{\dagger} c_{ilm'\sigma} c_{ilm-\sigma}$$

kinetic part, determined from DFT-LDA calculation (material specific)

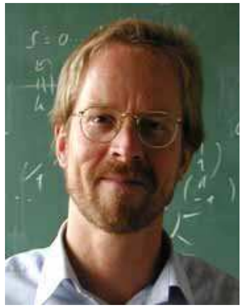
$$H_{LDA}^{0} = \sum_{ilm, jl'm', \sigma} t_{ilm, jl'm'}^{0} c_{ilm\sigma}^{\dagger} c_{jl'm'\sigma}$$

LDA+DMFT - state of the art for realistic approach to correlated electron systems

DMFT scheme

S_{loc} - local interactions U or J from a model **TB** or a microscopic **LDA** Hamiltonian

D. Vollhardt



W. Metzner

$$\hat{G} = -\langle T\hat{C}(\tau)\hat{C}^*(0)\rangle_{S_{loc}}$$

DMFT

$$\hat{\mathcal{G}}^{-1} = \hat{G}^{-1} + \hat{\Sigma} \qquad \hat{\Sigma} \qquad \hat{\Sigma} = \hat{\mathcal{G}}^{-1} - \hat{G}^{-1}$$

G. Kotliar

A. Georges

$$\hat{G} = \sum[(\omega+\mu)\hat{1} - \hat{H}^0 - \hat{\Sigma}]^{-1}$$

$\hat{H}^0$ is a model **TB** or a microscopic **LDA** Hamiltonian

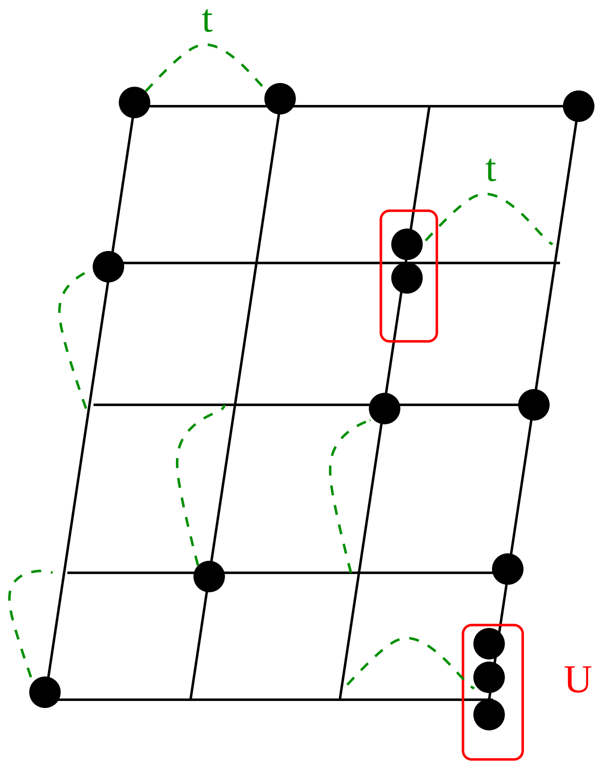
BOSONS

Correlated bosons on optical lattices

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

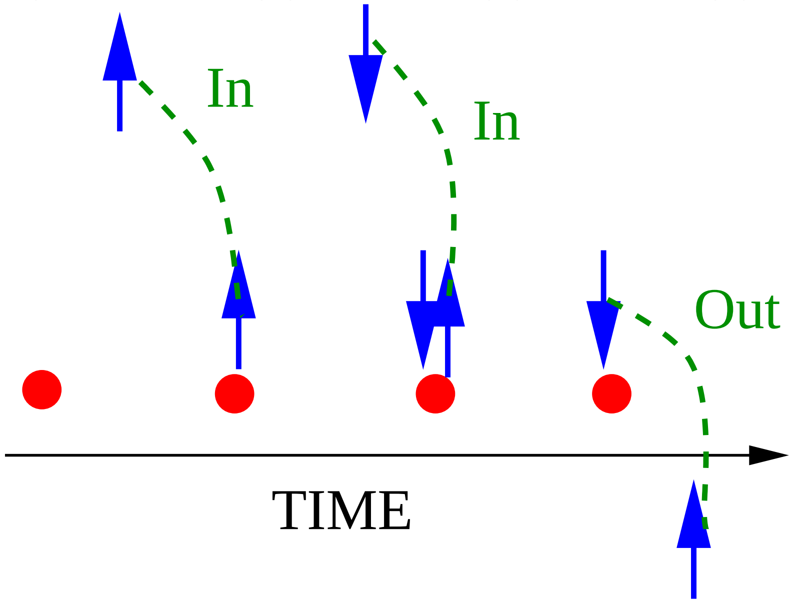
bosonic Hubbard model

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



local (on-site) correlations in time

$$E_{\mathrm{int}} = \quad U \qquad 3U \qquad 6U \qquad 3U$$



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

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 bosons in $d \to \infty$ limit

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

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

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

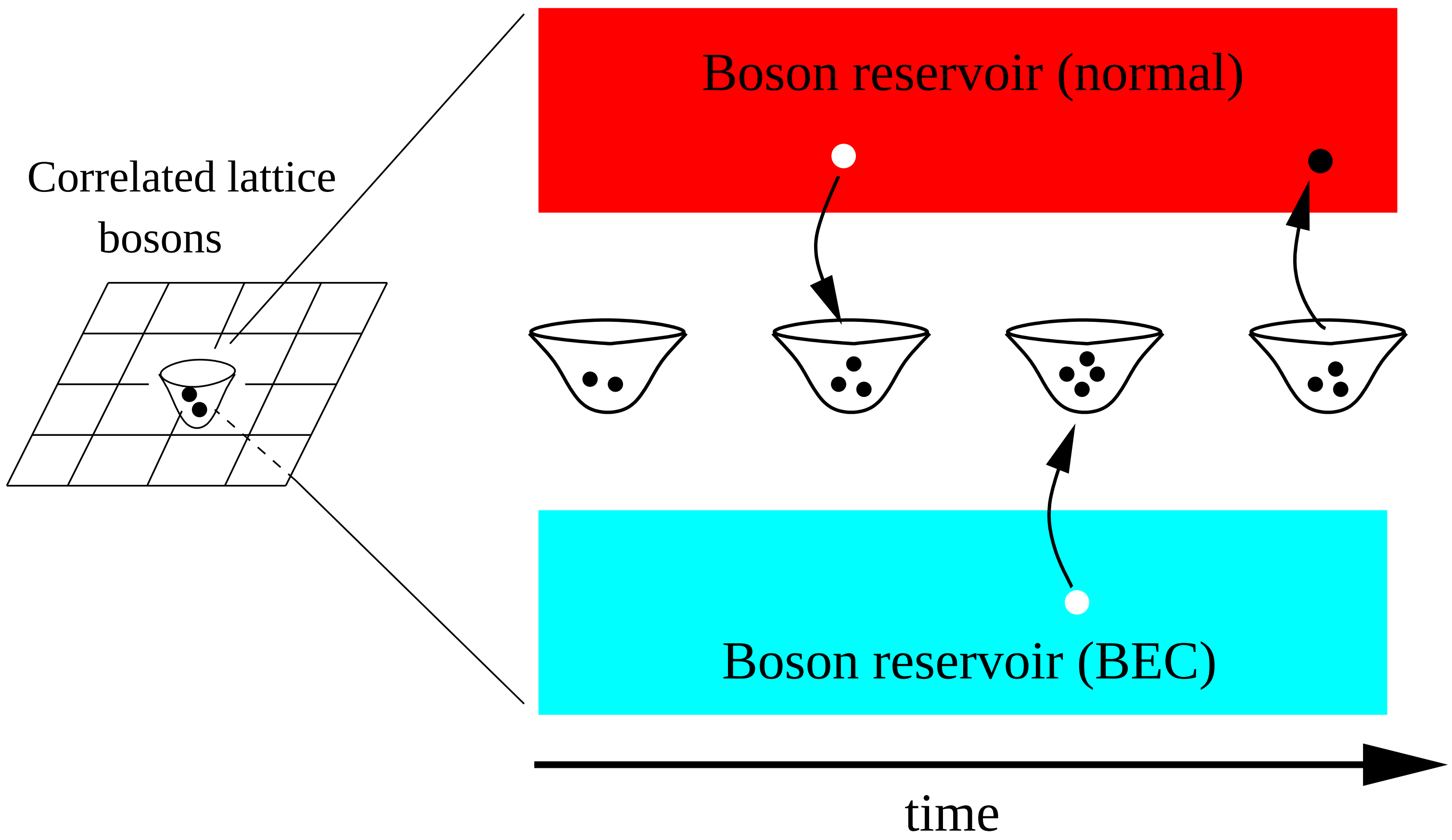
   - normal parts: $t_{ij} = \frac{t^*_{ij}}{(2d)^{\frac{||R_i - R_j||}{2}}}$ - fractional rescaling
   - BEC parts: $t_{ij} = \frac{t^*_{ij}}{(2d)^{||R_i - R_j||}}$ - integer rescaling

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

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

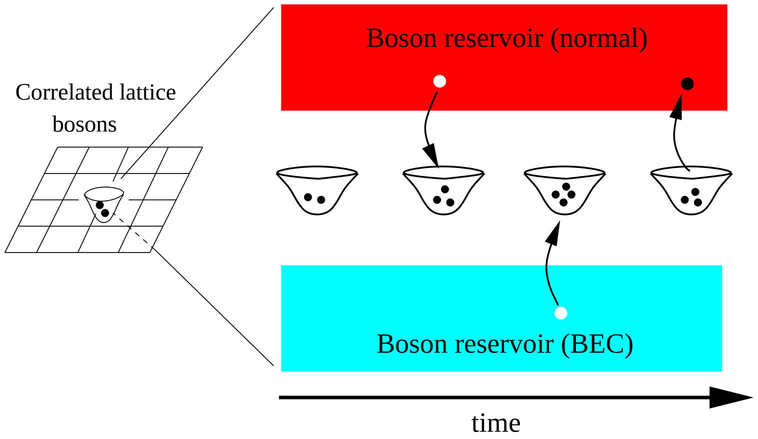
- Exact mapping of the lattice bosons in infinite dimension onto a single site
- Single site coupled to two reservoirs: normal bosons and bosons in the condensate
- Reservoirs properties are determined self-consistently, local correlations kept



B-DMFT application to bosonic Hubbard model

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

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



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

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

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

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

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

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

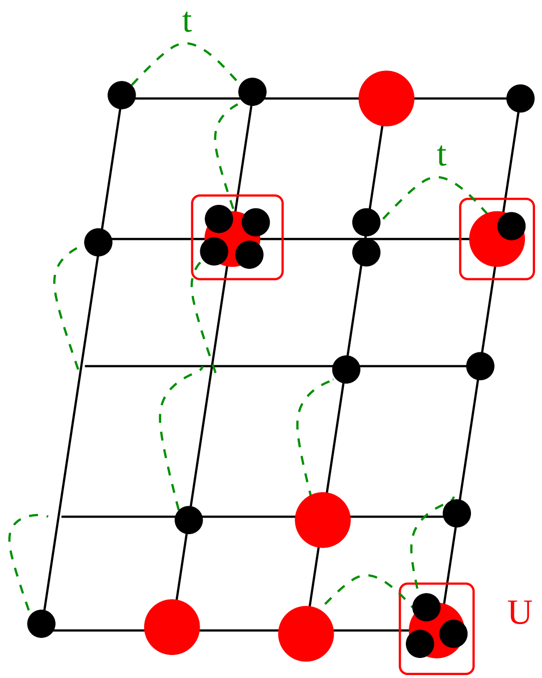
B-DMFT application to bosonic Falicov-Kimball model

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

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

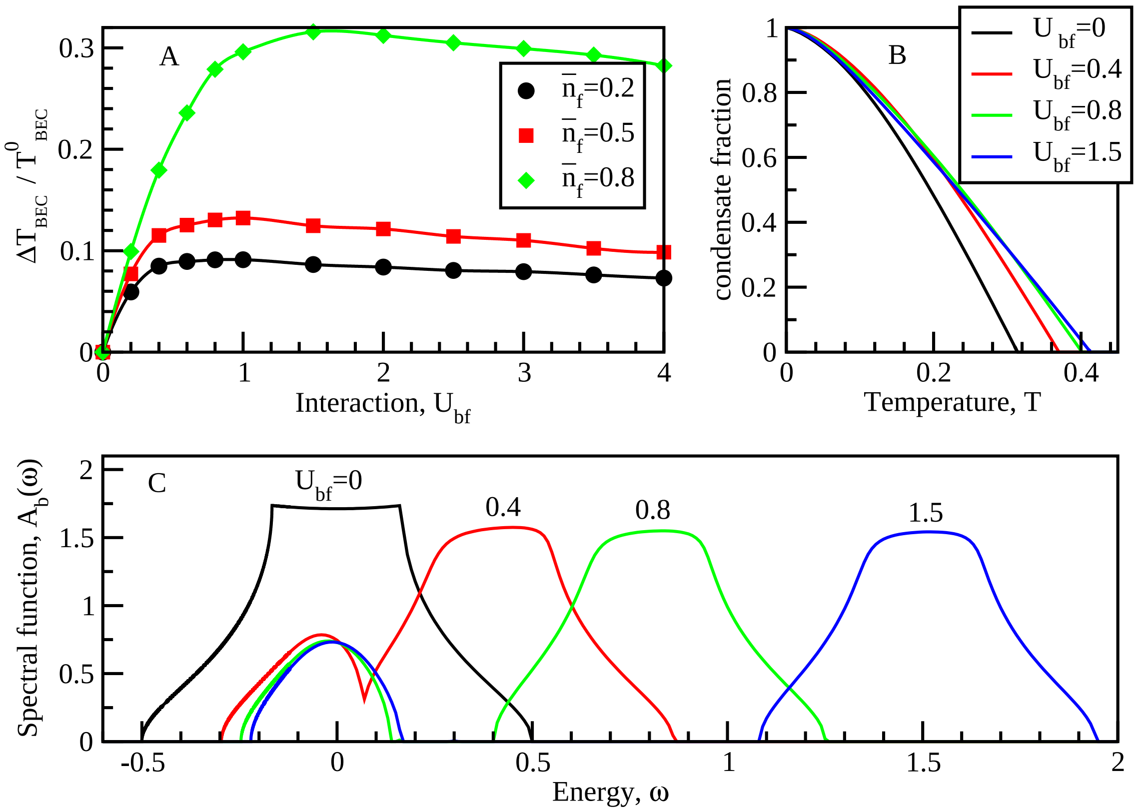
Local conservation law $[n_{fi}, H] = 0$ hence $n_{fi} = 0, 1, 2, \ldots$ classical variable

B-DMFT: local action Gaussian and analytically integrable



Enhancement of T_{BEC} due to interaction

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



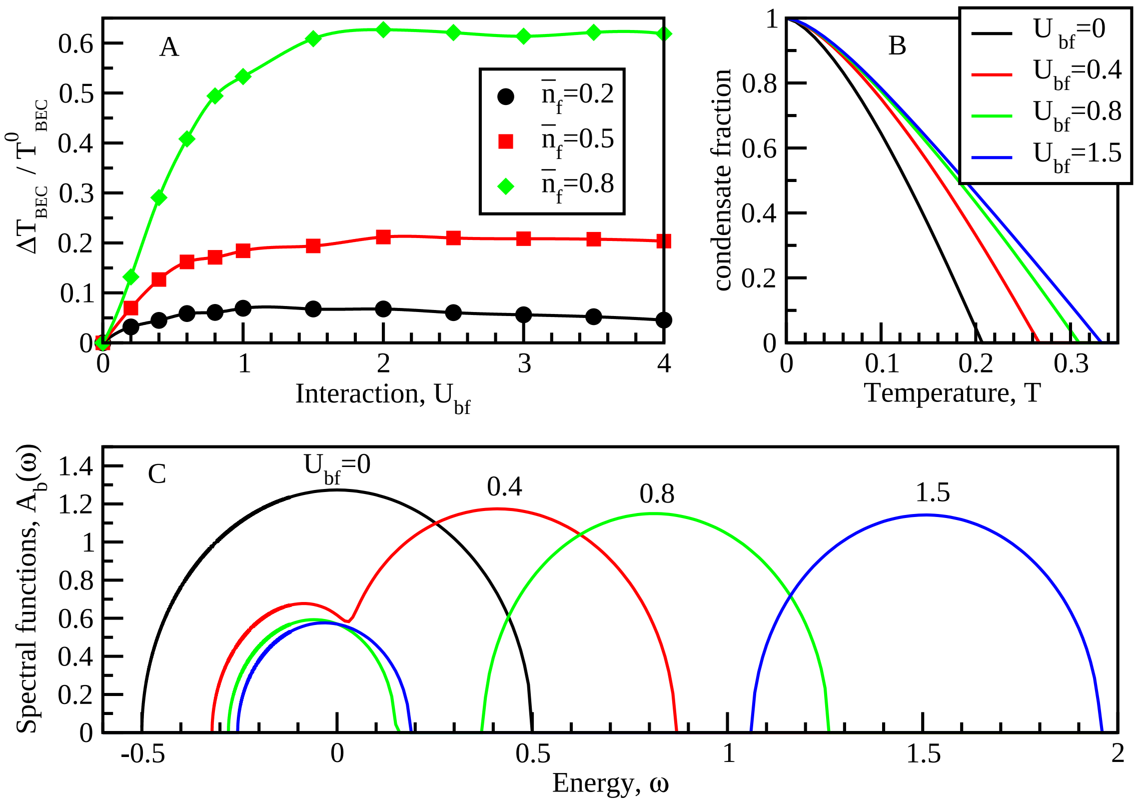
$$A_b(\omega) = -\mathrm{Im}G_b(\omega)/\pi$$

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

Normal part decreases when U increases for constant μ_b and T

Exact limit: enhancement of T_{BEC} due to interaction

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



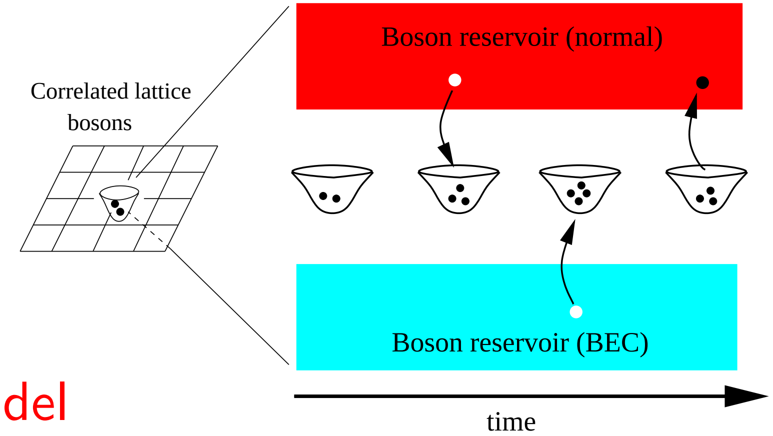
$$A_b(\omega) = -\mathrm{Im} G_b(\omega)/\pi$$

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

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 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