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

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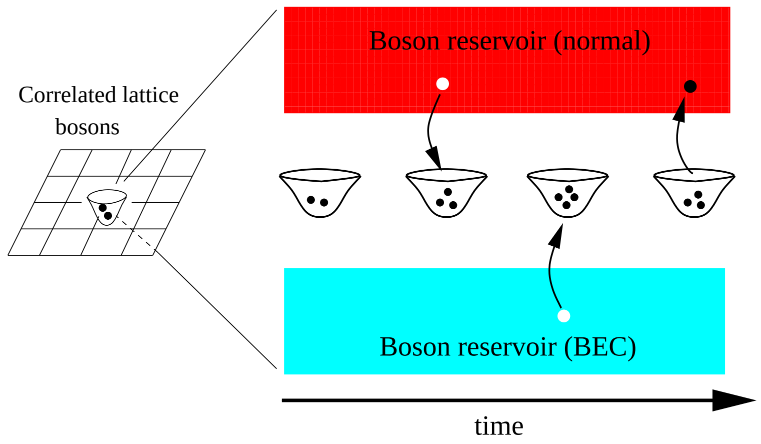
May 14th, 2008

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
- DMFT for bose-fermi mixtures
- Real-space formulation of DMFT

Collaboration

Dieter Vollhardt - Augsburg University

Correlated bosons on a lattice: Dynamical mean-field theory for Bose-Einstein condensed and normal phases - arXiv:0706.0839, accepted to Phys. Rev. B (2008)

Plan of talk

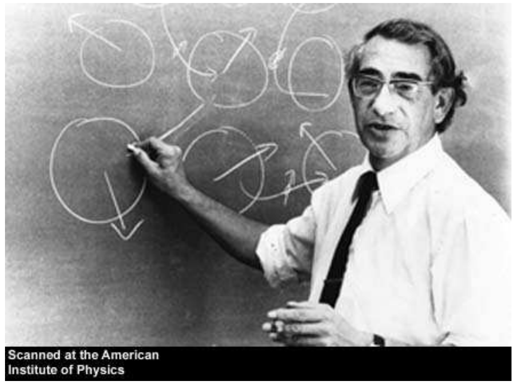
- Dynamical mean-field theory (DMFT) for correlated fermions
- Formulation of dynamical mean-field theory for bosons (B-DMFT)
- Bosonic Hubbard model within B-DMFT
- Falicov-Kimball model within B-DMFT
  - Enhancement of BEC transition temperature due to correlations
- Mixtures of bosons and fermions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

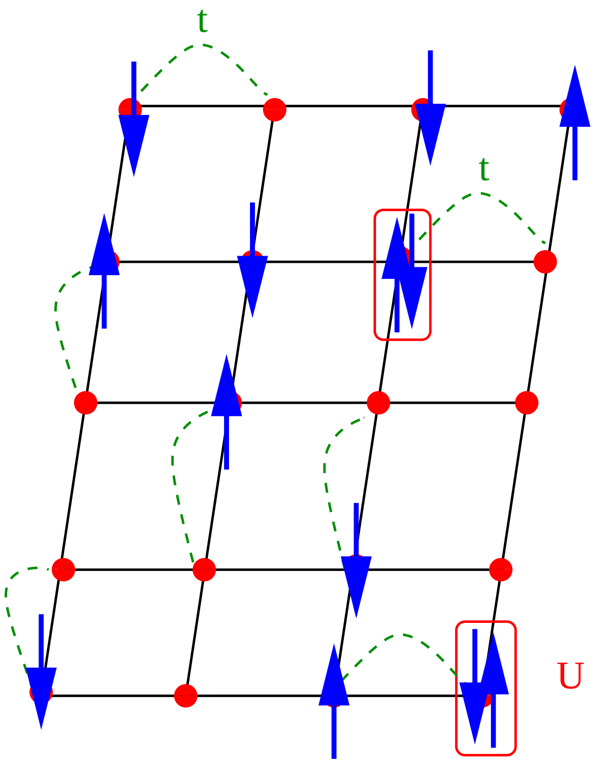
FERMIONS

Correlated lattice fermions

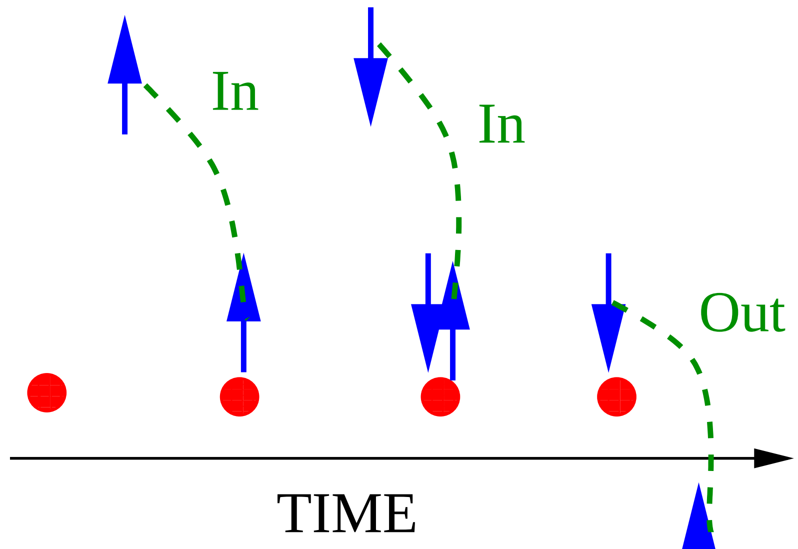
$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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

Fermions in large dimensions

Large dimensional limit is not unique

No scaling at all:

$$t_{ij} = t_{ij}, \quad U = U, \quad \text{etc.}$$

$$\frac{1}{N_L} E_{kin} = \frac{1}{N_L} \sum_{ij\sigma} t_{ij} \langle c^\dagger_{i\sigma} c_{j\sigma} \rangle = \infty\ !$$

Overscaling fermions

$$t_{ij} = \frac{t^*_{ij}}{d^{||\mathbf{R}_i - \mathbf{R}_j||}}, \quad U = U, \quad \text{etc.}$$

$$\frac{1}{N_L} E_{kin} = \frac{1}{N_L} \sum_{ij\sigma} t_{ij} \langle c^\dagger_{i\sigma} c_{j\sigma} \rangle = 0\ !$$

Fermions in large dimensions (coordination)

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

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

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

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

with rescaling

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

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

Comprehensive mean-field theory for fermions

$$H = H^{\text{hopping}} + H_{\text{loc}}^{\text{interaction}}$$

- comprehensive (all input parameters, temperatures, all phases, ...)
- thermodynamically consistent and conserving
- provides exact solutions in certain non-trivial limit (large d)

$$\langle H \rangle, \quad \langle H^{\text{hopping}} \rangle, \quad \langle H_{\text{loc}}^{\text{interaction}} \rangle$$

are finite and generically non-zero, and

$$\langle \left[H^{\text{hopping}}, H_{\text{loc}}^{\text{interaction}} \right] \rangle \neq 0$$

to describe non-trivial competition

Non-comprehensive mean-field theory for fermions

- Distance independent hopping (van Dongen, Vollhardt 92)

$$H = t \sum_{ij\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- Distance independent interaction (Spalek, Wojcik 88, Baskaran 91, Kohmoto 95, Gebhard 97)

$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{ij} n_{i\uparrow} n_{j\downarrow} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + U \sum_{\mathbf{k}} n_{\mathbf{k}\uparrow} n_{\mathbf{k}\downarrow}$$

In both models a non-trivial competition is suppressed

$$\langle \left[H^{\text{hopping}}, H^{\text{interaction}}_{\text{loc}} \right] \rangle = 0$$

although $\langle H \rangle, \quad \langle H^{\text{hopping}} \rangle, \quad \langle H^{\text{interaction}}_{\text{loc}} \rangle \neq 0$

$d \to \infty$ 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

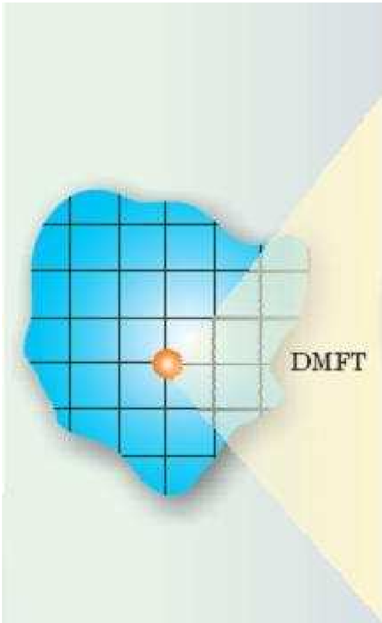
$$\Sigma_{\sigma}(\mathbf{k}, \omega_n) \to_{d\to\infty} \Sigma_{\sigma}(\omega_n)$$

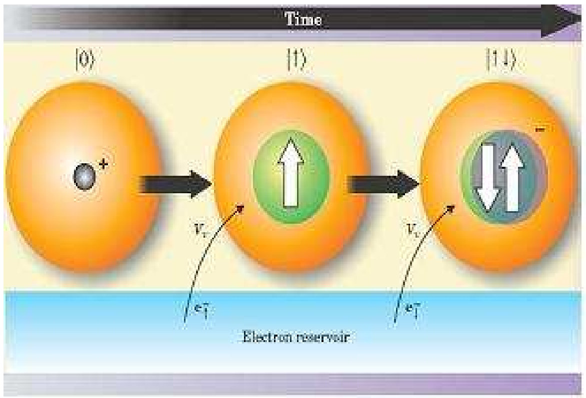
DMFT is an exact theory in infinite dimension (coordination number)
and a small control parameter is $1/d$ $(1/z)$

(Metzner, Vollhardt, 1989; Muller-Hartmann, 1989; Georges, Kotliar, 1990'; Janis, Vollhardt 1990', ...)

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 – flexibility; LDA+DMFT

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

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

direct and exchange interaction

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

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

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

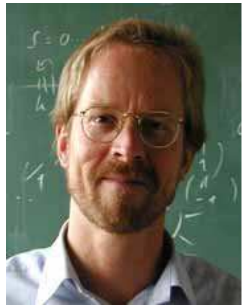
$$H^{0}_{LDA} = \sum_{ilm, jl'm', \sigma} t^{0}_{ilm, jl'm'} c^{\dagger}_{ilm\sigma} c_{jl'm'\sigma}$$

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

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



D. Vollhardt

W. Metzner

DMFT

$$\hat{\Sigma}$$

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

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

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

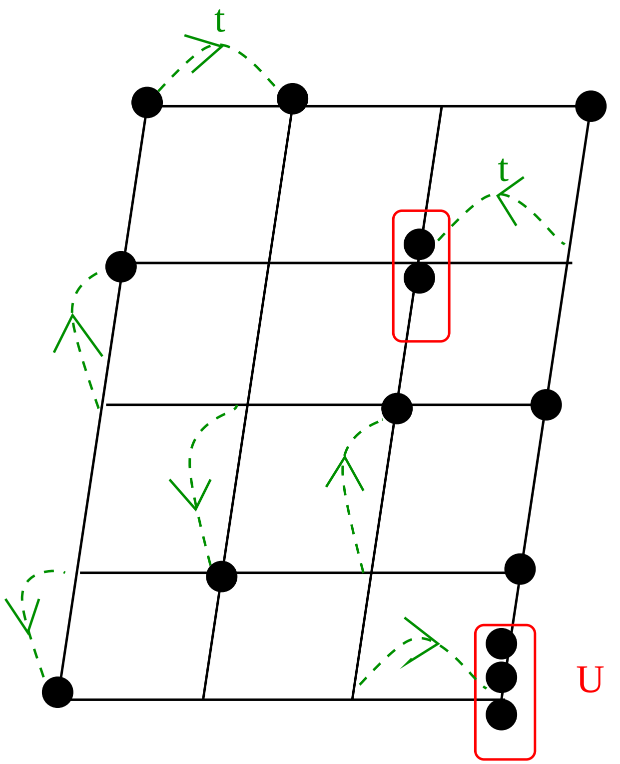
BOSONS

Correlated bosons on optical lattices

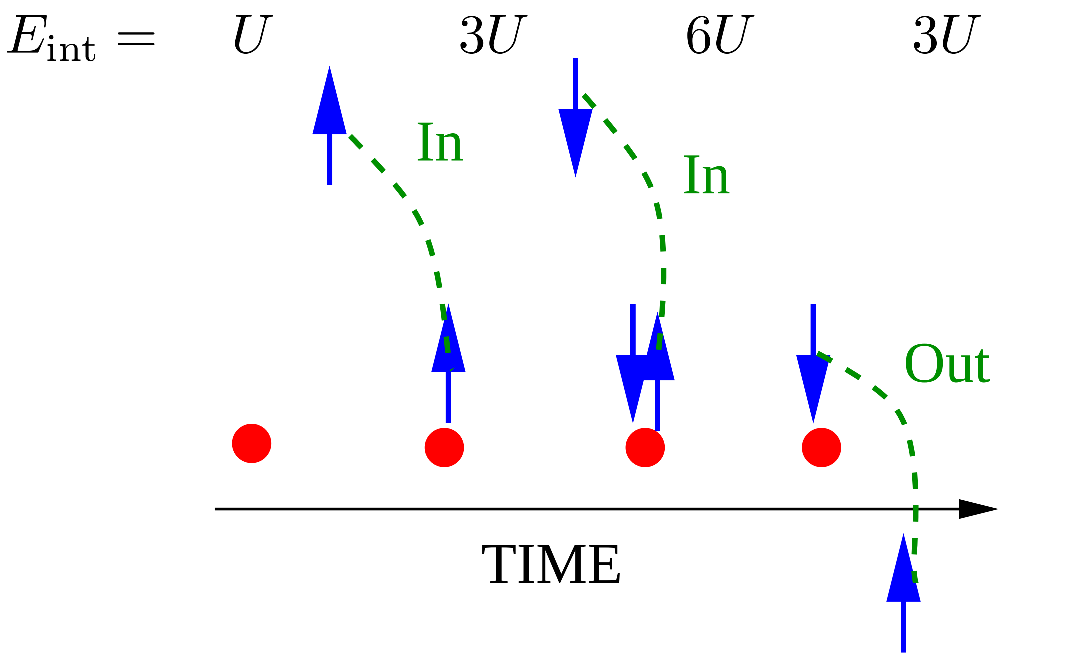
Gersch, Knollman, 1963
Fisher et al., 1989
Scalettar, Kampf, et al., 1995
Jacksch, 1998

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



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

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

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

- No scaling:

$$\frac{1}{N_L} E_{kin} = \infty$$

- Fractional scaling:

$$\frac{1}{N_L} E_{kin} = \infty$$

  in the BEC phase

- Integer scaling:

$$\frac{1}{N_L} E_{kin} = 0$$

  in the normal phase

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

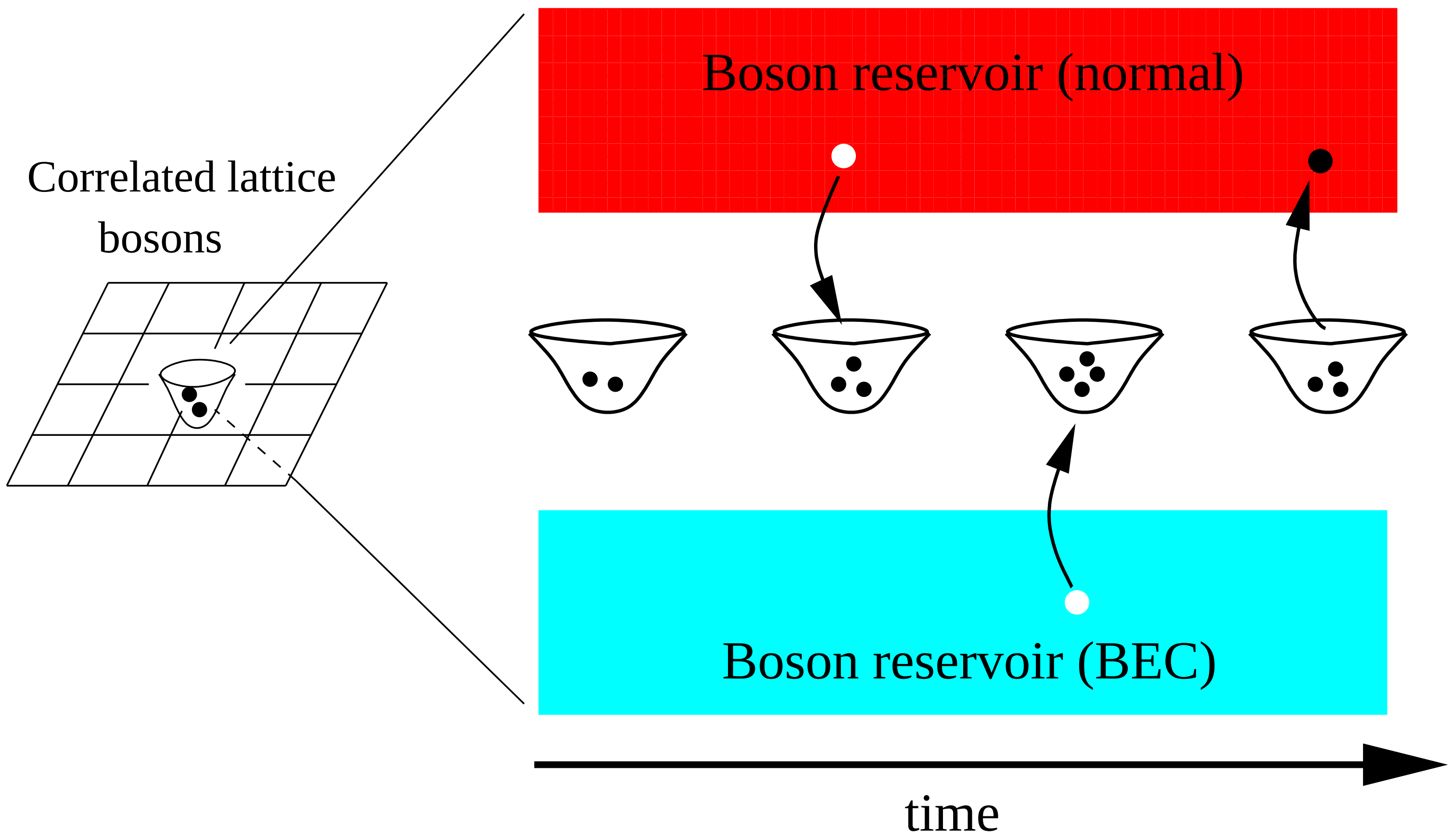
   - normal parts: $t_{ij} = \frac{t_{ij}^*}{(2d)^{\frac{||R_i - R_j||}{2}}}$ - fractional rescaling
   - BEC parts: $t_{ij} = \frac{t_{ij}^*}{(2d)^{||R_i - R_j||}}$ - integer rescaling

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

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

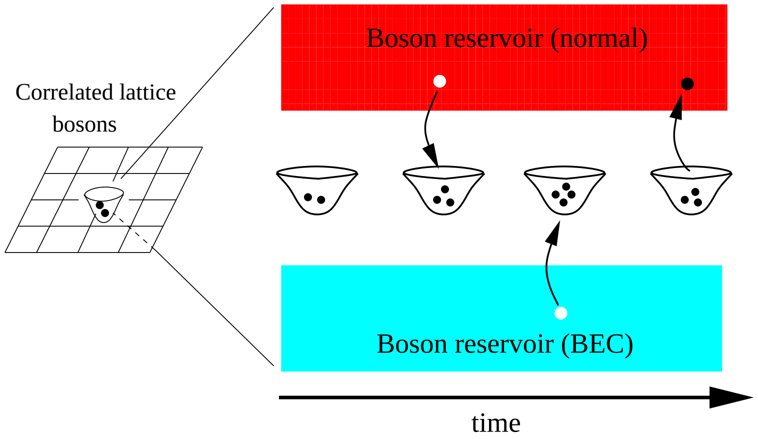
- Exact mapping of the lattice bosons in infinite dimension onto a single site
- Single site coupled to two reservoirs: normal bosons and bosons in the condensate
- Reservoirs properties are determined self-consistently, local correlations kept



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

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

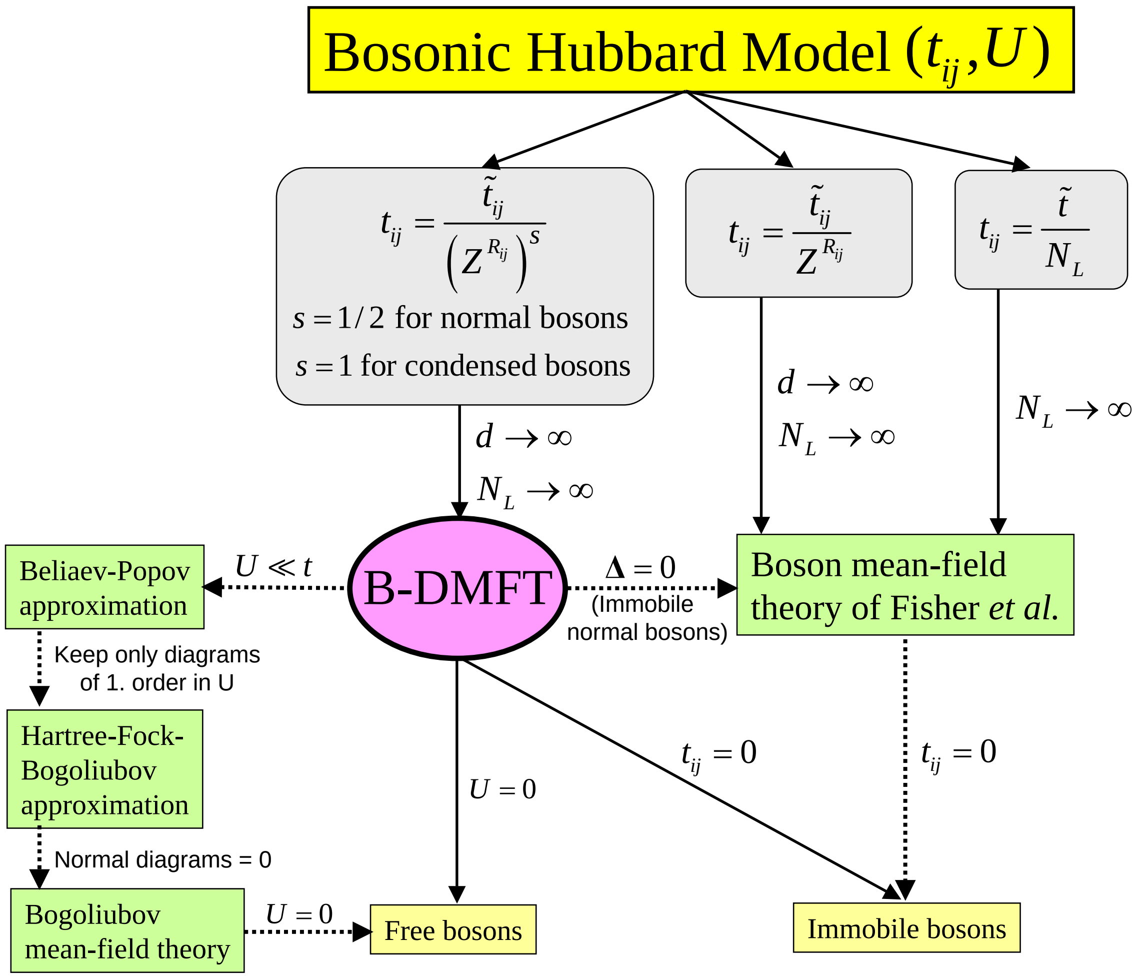
$$\kappa \int_0^\beta d\tau \bar{\phi}^\dagger(\tau)\bar{b}(\tau) + \frac{U}{2} \int_0^\beta n(\tau)(n(\tau) - 1)$$

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

(iii) Condensate wave function

$$\bar{\phi}(\tau) = \int D[b^*, b]\ \bar{b}(\tau)\ e^{-S_{loc}}$$

B-DMFT in well-known limits



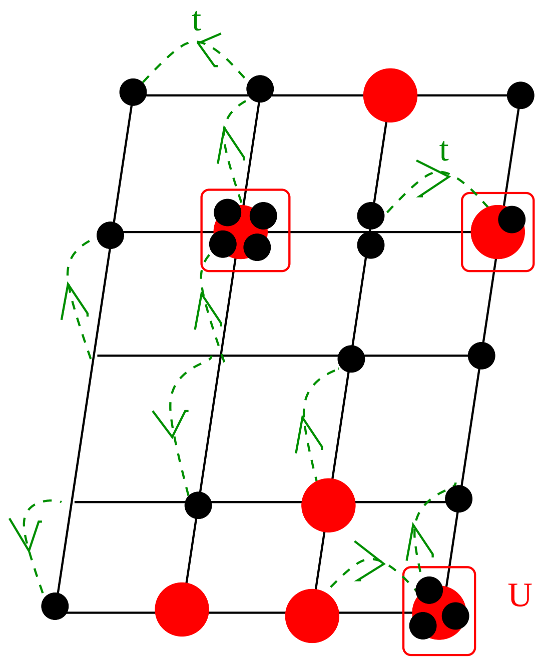
B-DMFT application to bosonic Falicov-Kimball model

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

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

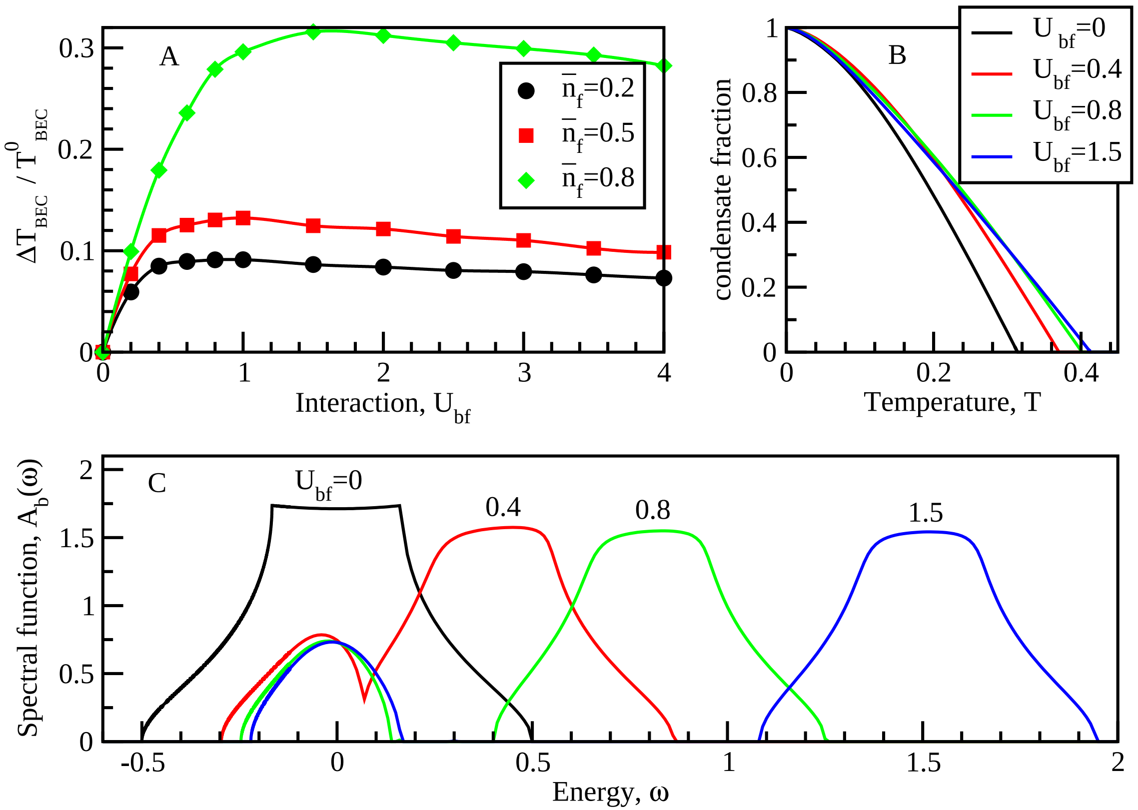
Local conservation law $[n_{fi}, H] = 0$ hence $n_{fi} = 0, 1, 2, ...$ classical variable

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



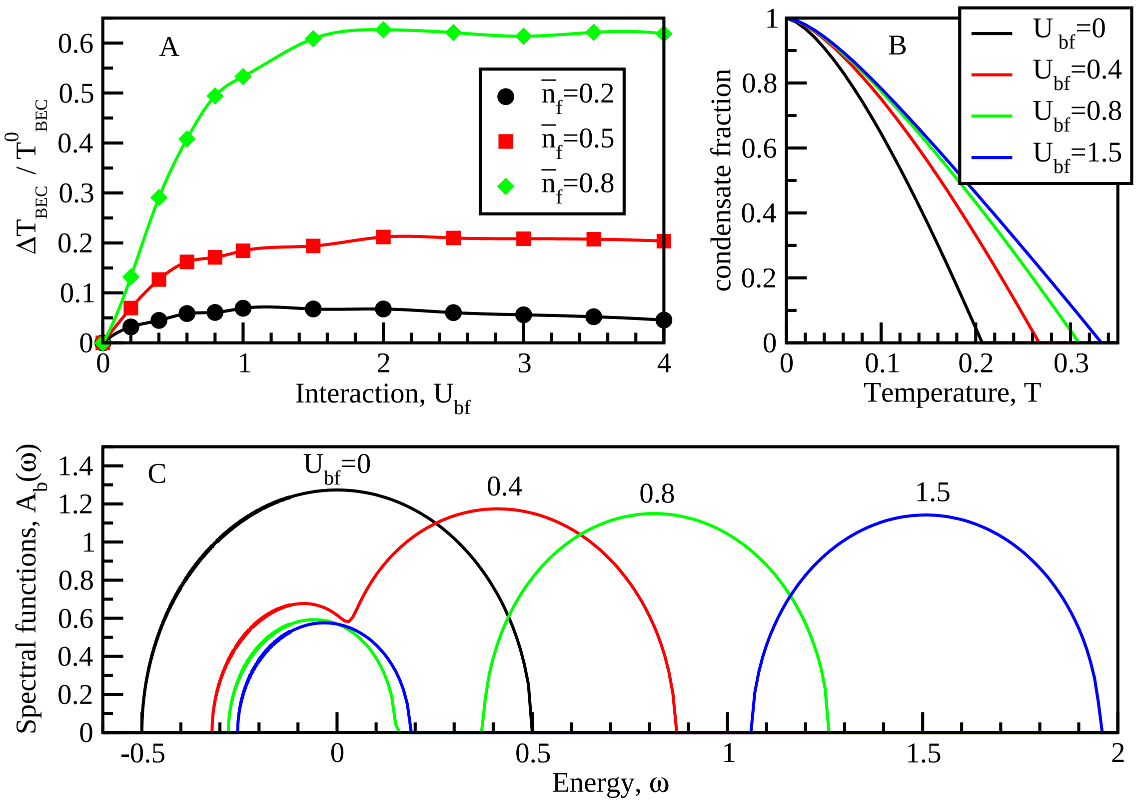
$$A_b(\omega) = -\mathrm{Im}G_b(\omega)/\pi$$

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

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 $U_{ff} = \infty$; $n_f = 0, 1$; $0 \leq \bar{n}_f \leq 1$; $d = \infty$ - Bethe lattice



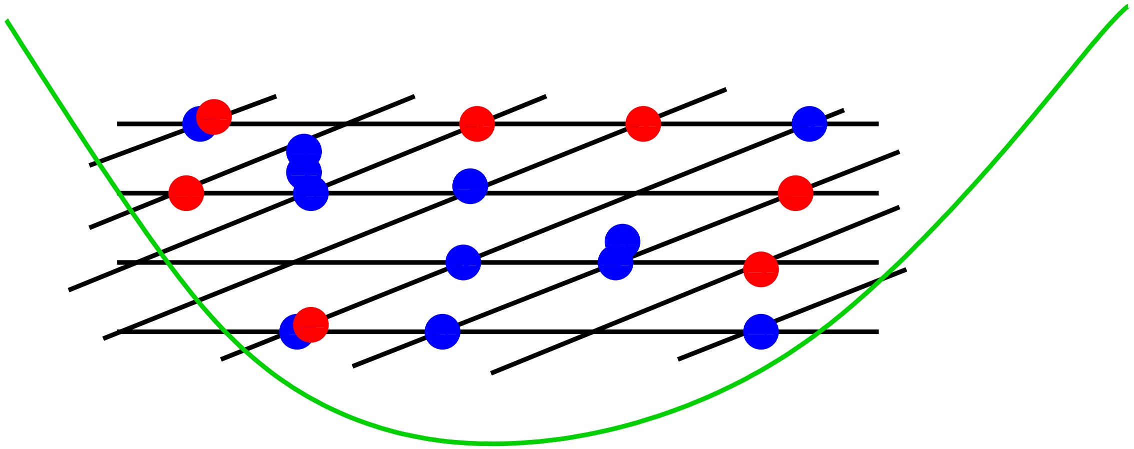
$$A_b(\omega) = -\mathrm{Im} G_b(\omega)/\pi$$

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

Normal part decreases when U increases for constant μ_b and T

Bose-Fermi mixtures (^{87}Rb-^{40}K) on a lattice with 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:

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

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

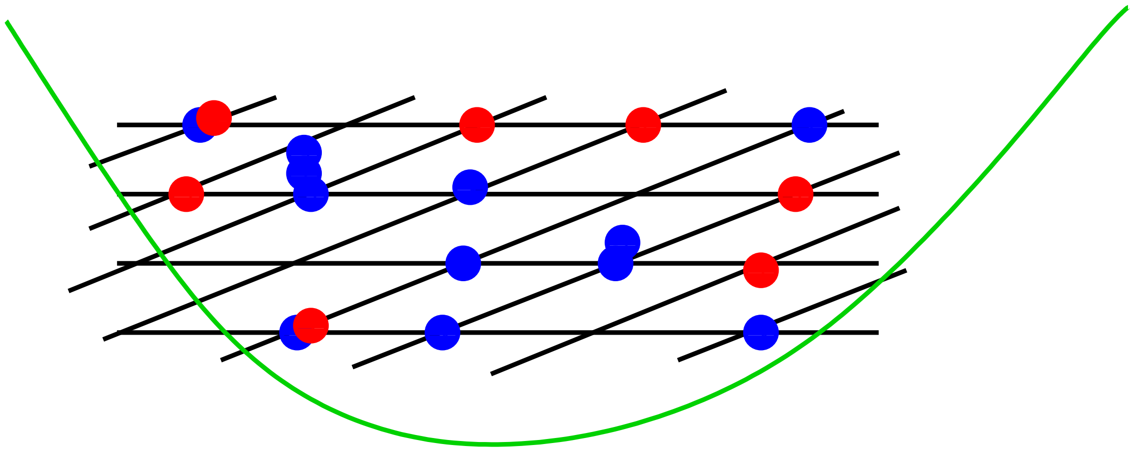
$$S_{i_0}^{\mathrm{f}} = \int_0^\beta d\tau f_{i_0}^*(\tau) \left(\partial_\tau - \mu_f + \epsilon_{i_0}^f\right) f_{i_0}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' f_{i_0}^*(\tau) \Delta_{i_0}^f(\tau - \tau') f_{i_0}(\tau')$$

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

Lattice self-consistency (Dyson) equations

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

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



Integrating out fermions

$$Z_{i_0}^{\mathrm{loc}} = \int D[b] e^{-S_{i_0}^{\mathrm{b}}[b] + \ln \mathrm{Det}\left[M_{i_0}^b\right]}$$

$$[M_{i_0}^b]_{nm} \equiv \left[(\partial_\tau - \mu_f + \epsilon_{i_0}^f + U_{bf} n_{i_0}^b(\tau))\delta_{\tau,\tau'} + \Delta_{i_0}^f(\tau - \tau') \right]_{nm}$$

$$= \left[-i\omega_n - \mu_f + \epsilon_{i_0}^f + \Delta_{i_0}^f(\omega_n) \right] \delta_{nm} + \frac{U_{bf}}{\sqrt{\beta}} n_{i_0}^b(\omega_n - \omega_m)$$

Effective interaction between bosons

$$\ln \mathrm{Det}[M^b] = \mathrm{Tr}\ln[M^b] = \mathrm{Tr}\ln[-(\mathcal{G}^f)^{-1} + M_1^b] = \mathrm{Tr}\ln[-(\mathcal{G}^f)^{-1}] - \sum_{m=1}^{\infty} \frac{1}{m} \mathrm{Tr}[\mathcal{G}^f M_1^b]^m$$

$$\mathcal{G}_{i_0}^f(\omega_n) = \frac{1}{i\omega_n + \mu_f - \epsilon_{i_0}^f - \Delta_{i_0}^f(\omega_n)}$$

Effective bosonic action

$$\tilde{S}_{i_0}^b \approx S_{i_0}^b + \frac{U_{bf}}{\sqrt{\beta}} \sum_n \mathcal{G}_{i_0}^f(\omega_n) n_{i_0}^b(\nu_m = 0) - \frac{U_{bf}^2}{2} \sum_n n_{i_0}^b(\nu_n) \pi_{i_0}^f(\nu_n) n_{i_0}^b(-\nu_n)$$

$$\pi_{i_0}^f(\nu_n) \equiv -\frac{1}{\beta} \sum_m \mathcal{G}_{i_0}^f(\omega_m) \mathcal{G}_{i_0}^f(\omega_m + \nu_n)$$

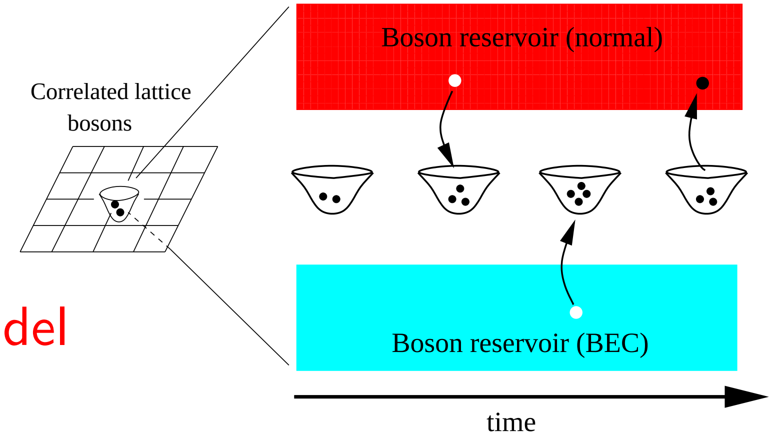
Boson-Boson interaction

$$U_b^{\text{eff}} = U_b - U_{bf}^2 N_{i_0}^f(\mu)$$

System unstable when $U_b = U_{bf}^2 N_{i_0}^f(\mu)$.

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

- Bosonic impurity solver wanted!