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

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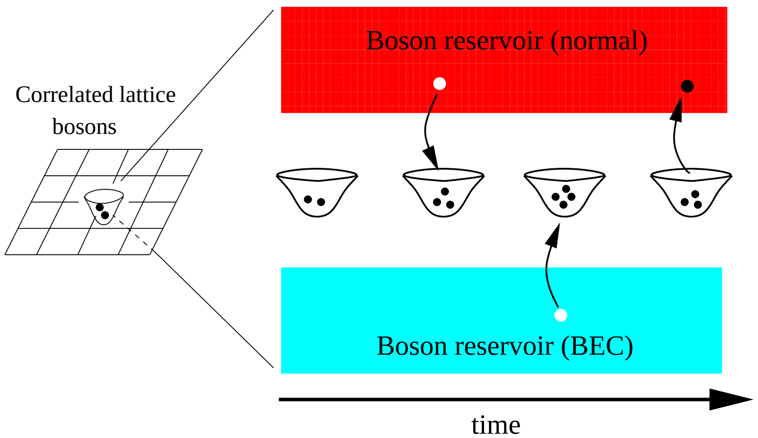
Main results

- 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
- 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

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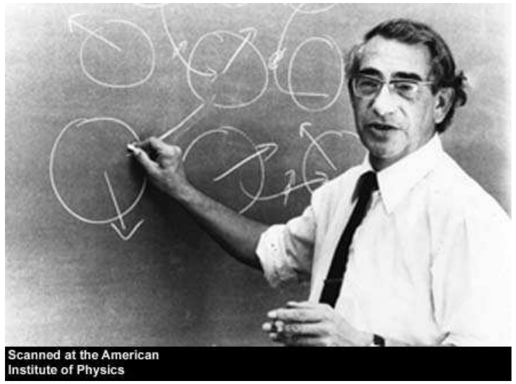
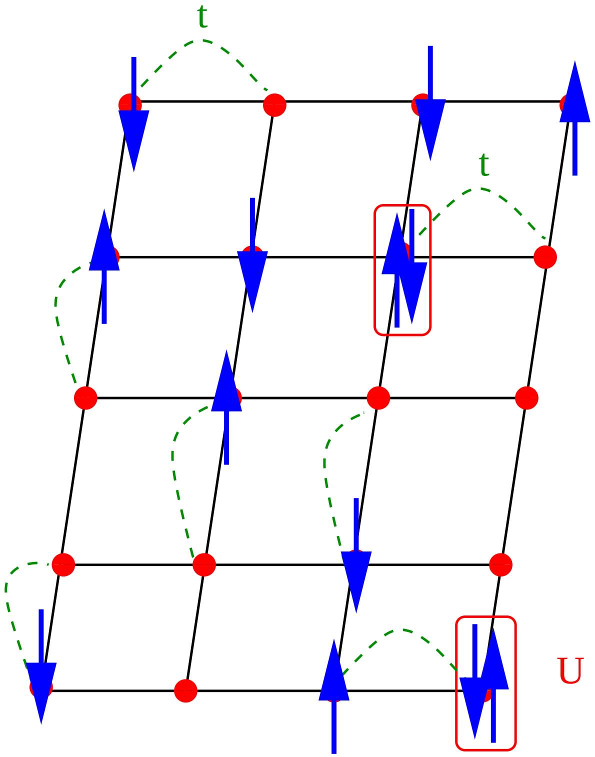
FERMIONS

Correlated lattice fermions

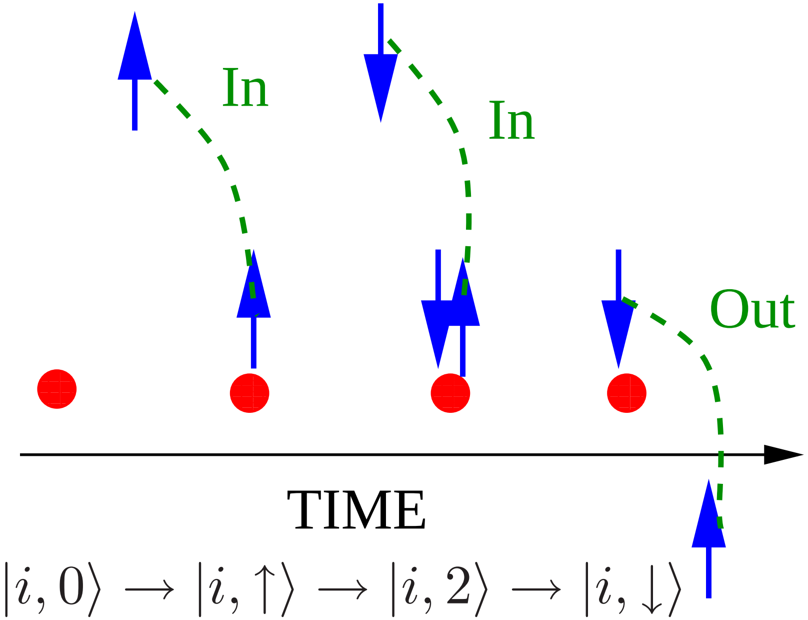
$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

fermionic Hubbard model, 1963





Local Hubbard physics



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

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

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

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)

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

- Distance independent interaction (Spalek, Wojcik 88, KB 92-94, Baskaran 91, Kohmoto 95, Gebhard 97)

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

In both models a non-trivial competition is suppressed

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

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

$d \to \infty$ 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

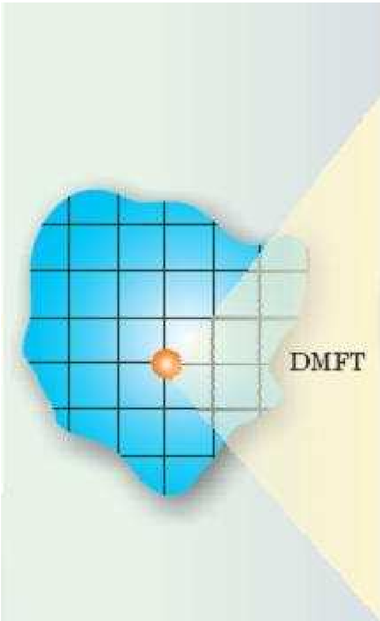
$$\Sigma_\sigma(\mathbf{k}, \omega_n) \to_{d\to\infty} \Sigma_\sigma(\omega_n)$$

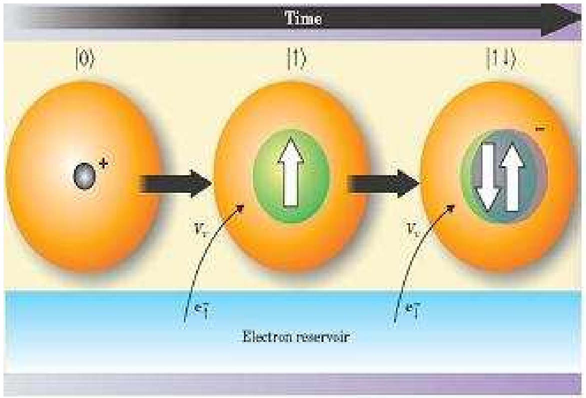
DMFT is an exact theory in infinite dimension (coordination number)
and a small control parameter is $1/d$ $(1/z)$

(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, ...)

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

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)

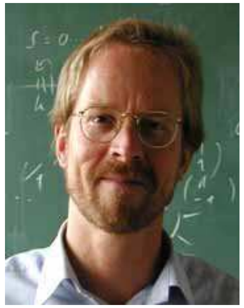
$$H_{LDA}^{0} = \sum_{ilm, jl'm', \sigma} t_{ilm, jl'm'}^{0} c_{ilm\sigma}^{\dagger} c_{jl'm'\sigma}$$

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

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



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

Short-history: Bose-Einstein distribution

- M. Planck 1900 - introduces distingushable quanta of energy and gets BE function

$$\bar{\epsilon}(\omega) = \sum_{n=0}^{\infty} \hbar\omega n e^{\frac{\hbar\omega}{k_B T} n} = \frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1}.$$

- L. Natanson 1911 - introduces concept of indistingushable photon quanta and by combinatorial way gets BE distribution function

$$n_\epsilon = \frac{1}{e^{\frac{\epsilon}{k_B T}} - 1},$$

  in *On the statistical theory of Radiation*, Bulletin de l'Académie des Sciences de Cracovie (A), 134 (1911); German translation in Phys. Z. **12**, 659 (1911).

- S.N. Bose 1924 - independently gets BE distribution function, paper rejected from Phil. Mag. and after translation by Einstein published in Z. Phys. **26**, 178 (1924).

74 Wł. Natanson.

$$\frac{E}{N} = \tfrac{3}{2} kT; \qquad (13)$$

zatem istotnie, jak powinniśmy byli otrzymać, wielkość $\tfrac{3}{2}kT$ jest średnią kinetyczną energią cząsteczki gazu doskonałego o temperaturze T. Por. § 32.

§ 52. **Teorya Plancka. Drugie główne twierdzenie.** Przyjmujemy teraz równanie (8) § 49-go, czyli twierdzenie Boltzmanna. Zamiast znaku $\mathfrak{A}$ wstawiamy wartość największą, którą osiąga wielkość, dana przez formułę (5) § 39-go. Ze względu na równania (7) i (8) § 38-go oraz (6) § 43-go otrzymujemy, co następuje:

$$S = k\{N \log N - N \log N_0 - n \log x\} + \text{const.}, \qquad (1)$$

gdzie stała dodatkowa nie powinna zależeć od n.

Wzór (1) jest ogólny. Przejdźmy teraz do uważania dwóch przypadków szczególnych, o których mówiliśmy w artykułach 46 i 47. Przypuśćmy po pierwsze, że Q § 46-go jest bardzo małym, znacznie od jedności mniejszym ułamkiem. Z § 47-go wiadomo, że popełnimy bardzo mały błąd, jeżeli położymy w tym razie

$$x = \frac{Q}{1+Q}; \quad N_0 = \frac{N}{1+Q}. \qquad (2)$$

Z powyższego równania (1) wyprowadzamy podówczas:

$$S = k\{(n+N)\log(n+N) - n \log n - N \log N\} + \text{const.} \qquad (3)$$

Według (8) § 48-go mamy jednakże, w stanie równowagi:

$$\frac{\partial S}{\partial n} = \frac{\varepsilon}{T}. \qquad (4)$$

Z (3) i (4) wypada natychmiast:

$$Q = \frac{n}{N} = \frac{E}{N\varepsilon} = \frac{1}{e^{\varepsilon/kT} - 1}, \qquad (5)$$

gdzie e jest podstawą logarytmów naturalnych. Z tego równania (5), które nazywamy *drugiem głównem równaniem* Teoryi, otrzymamy niebawem formułę promieniowania, odkrytą przez Plancka.

Przypominamy obecnie z § 47-go, że, jeżeli Q jest mała, wartość (x) leży pomiędzy ówczesną a oraz Q. Zatem, ażeby uzyskać równanie (5) Plancka, musieliśmy przyjąć za (x) jego dolną granicę. Jeżeli do równania (1) wstawimy zamiast (x) jego górną granicę, t. j. jeżeli założymy

Rys. 2. Strona monografii [5] z jawnym wyrażeniem na rozkład statystyczny dla liczby fotonów n o energii $\varepsilon = \hbar\omega$ przy N dostępnych stanach (funkcja wykładnicza ma tu symbol ε). Zauważmy także wzór (3) na entropię bozonów o zadanej energii $\hbar\omega$ (wynik dla całkowitej entropii jest podany jako wzór (32) w obecnym artykule).

Ponadto, liczba rozkładów wspólnych dla N atomów (stanów) oraz n kwantów (fotonów), gdy fotony są nierozróżnialne, jest dana wzorem

$$U_\Sigma = \frac{(n+N-1)!}{n!(N-1)!}. \qquad (15)$$

Symbol U_Σ oznacza tu sumę liczb konfiguracji rozmieszczeń atomów z n fotonami oraz n fotonów pomiędzy atomami. Zauważmy od razu, że wzór powyższy ma taka samą postać jak wzór (8), lecz tam zamiast całkowitej liczby atomów mamy liczbę stanów g_i o danej energii ε_i. Podobna uwaga dotyczy n_i, zatem obecnie n musi odgrywać rolę średniej liczby fotonów w układzie (czy też wartości najbardziej prawdopodobnej). Widać teraz, dlaczego obecne podejście jest podejściem globalnym, w którym zadane są dwie liczby:

$$\sum_{i=0}^{p} N_i = N, \qquad (16)$$

$$\sum_{i=0}^{p} iN_i = n. \qquad (17)$$

Następnie wprowadzamy prawdopodobieństwo P obsadzenia rozważanego rozdziału energii. W tym celu definiujemy wielkość

$$P = \frac{U}{U_\Sigma} = \frac{N!n!(N-1)!}{(n+N-1)!}\left(\prod_{i=0}^{p} N_i!\right)^{-1}. \qquad (18)$$

Prawdopodobieństwo to opisuje typową konfigurację z n fotonami w układzie. Osiąga ono wartość maksymalną przy zadanych n oraz N, gdy iloczyn $\prod_{i=0}^{p} N_i!$ przyjmuje wartość minimalną. Stąd też cały problem sprowadza się do znalezienia warunkowego minimum

Władysław Natanson, 1864-1937

Teoria promieniowania (Theory of radiation) - 1912

Short-history: Bose-Einstein condensation (BEC)

A. Einstein 1925 - considers conserved bosons (μ defined) and observes that

$$N = \int_0^\infty d\epsilon \frac{N_0(\epsilon)}{e^{\frac{\epsilon-\mu}{k_B T}} - 1}$$

is *only* correct for $N \leq N_c = \zeta(3/2)(2\pi\hbar^2/mk_BT)^{3/2}$ in $d = 3$,
cf. Berl. Ber. **22**, 261 (1924), ibid. **23**, 3 and 18 (1925).

$$\frac{2\pi\hbar}{\sqrt{2mk_BT}} = \lambda_{dB} > a_0 = \left(\frac{N}{V}\right)^{-\frac{1}{d}}$$

Bose-Einstein Condensation: for conserved bosons above N_c (below T_c) the lowest energy state is occupied by macroscopicaly large number of bosons. Then $\mu = 0$ and the state $\epsilon_{\mathbf{k}=0}$ must be treated separately

$$N = N_c + \int_0^\infty d\epsilon \frac{N_0(\epsilon)}{e^{\frac{\epsilon}{k_B T}} - 1},$$

Short-history: general BEC as ODLRO

O. Penrose 1951, O. Penrose and L. Onsager 1956
Off-Diagonal Long Range Order (ODLRO) as a general definition of BEC for interacting bosons in any ensamble, external potential, etc.

one-particle reduced density matrix

$$\rho(r,r';t) \equiv N \sum_s p_s \int dr_2 ... dr_N \Psi_s^*(r r_2 .. r_N; t) \Psi_s(r' r_2 ... r_N; t) = \langle \psi^\dagger(rt) \psi(r't) \rangle$$

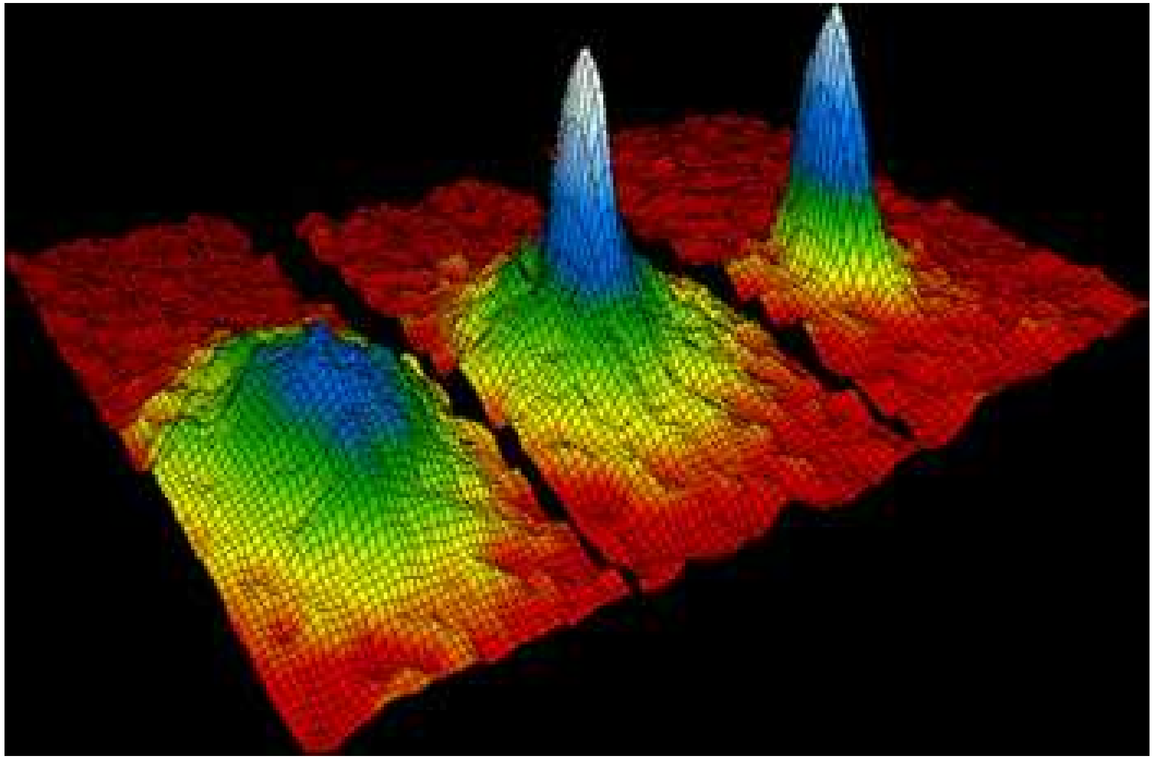
spectral decomposition (diagonalization)

$$\rho(r,r';t) = \sum_\alpha n_\alpha(t) \chi_\alpha^*(rt) \chi_\alpha(r't)$$

BEC occurs when there exists one-particle state(s) $\alpha = 0$ for which $n_0 = N_c \sim O(N)$

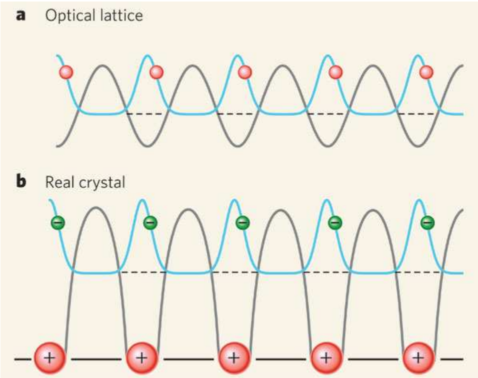
Short history: True experiments with BEC

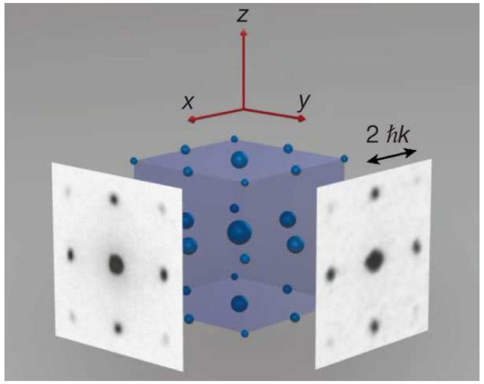
Magneto-optical traps with cold alkaline atoms with Bose statistics (^{7}Li, ^{23}Na, ^{41}K, ^{52}Cr, ^{85}Rb, ^{87}Rb, ^{133}Cs and ^{174}Yb)

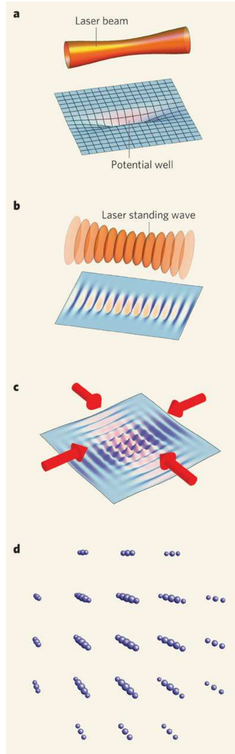


M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, 1995

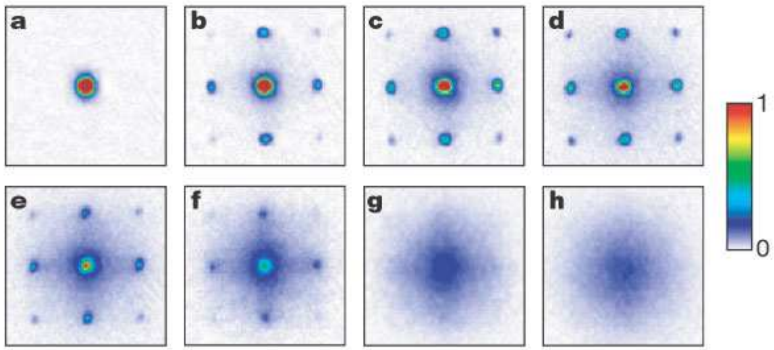
Short history: Superfluid-Mott transition

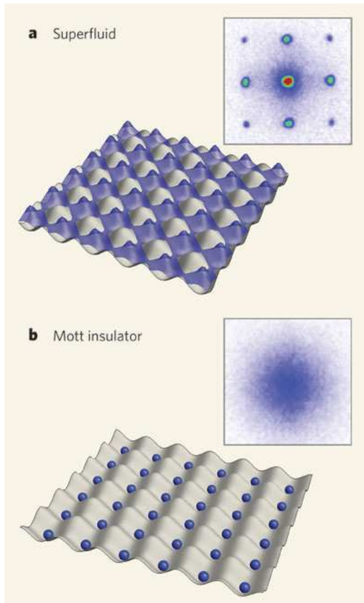






Optical lattices with cold atoms





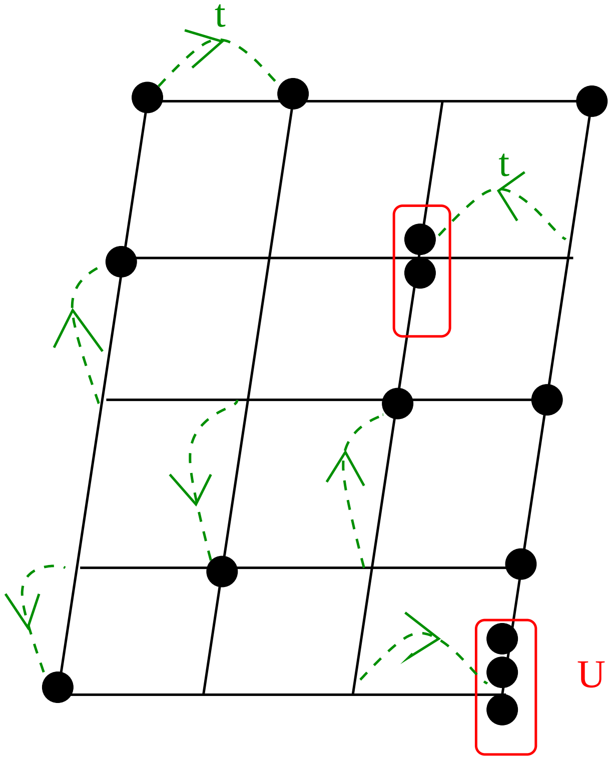
Superfluid-Mott insulator transition, Greiner, Mandel, Esslinger, Hänsch, Bloch, 2002

Correlated bosons on optical lattices

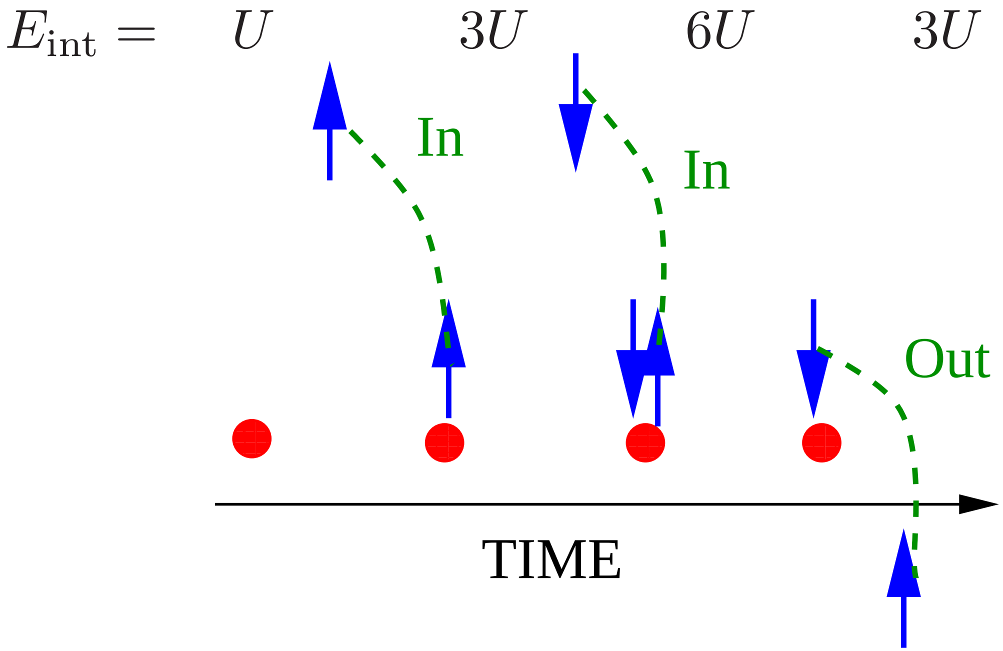
Gersch, Knollman, 1963
Fisher et al., 1989
Scalettar, Kampf, et al., 1995
Jacksch, 1998

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

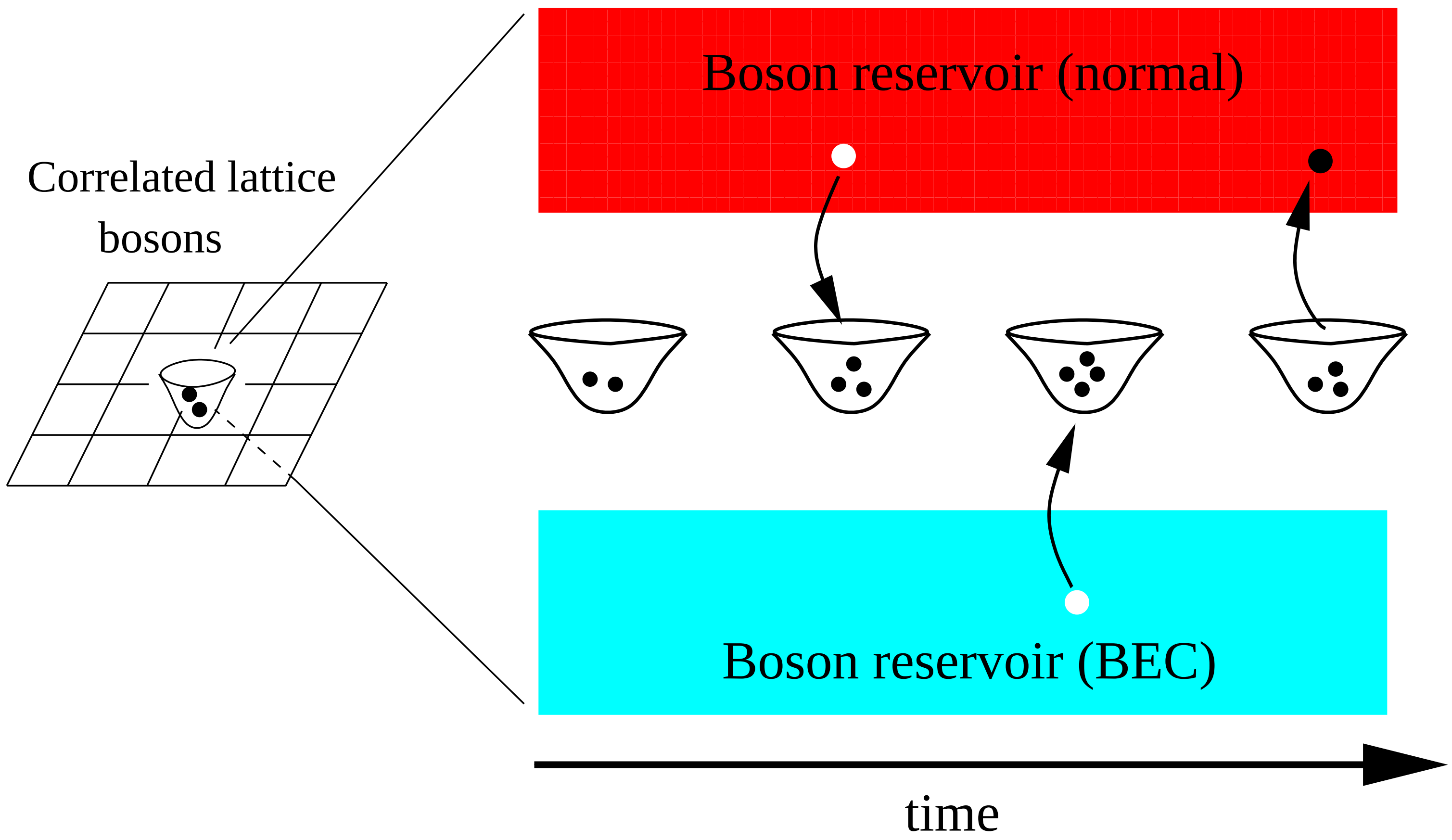
   - normal parts: $t_{ij} = \frac{t^*_{ij}}{(2d)^{\frac{||R_i - R_j||}{2}}}$ - fractional rescaling
   - BEC parts: $t_{ij} = \frac{t^*_{ij}}{(2d)^{||R_i - R_j||}}$ - integer rescaling

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)

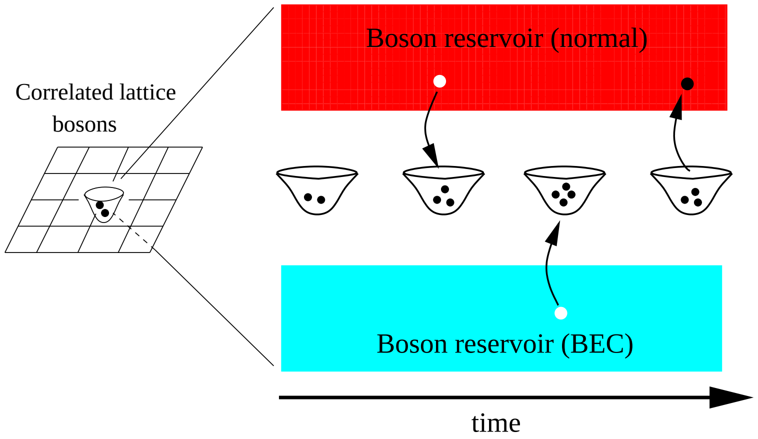
- Exact mapping of the lattice bosons in infinite dimension onto a single site
- Single site coupled to two reservoirs: normal bosons and bosons in the condensate
- Reservoirs properties are determined self-consistently, local correlations kept



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

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

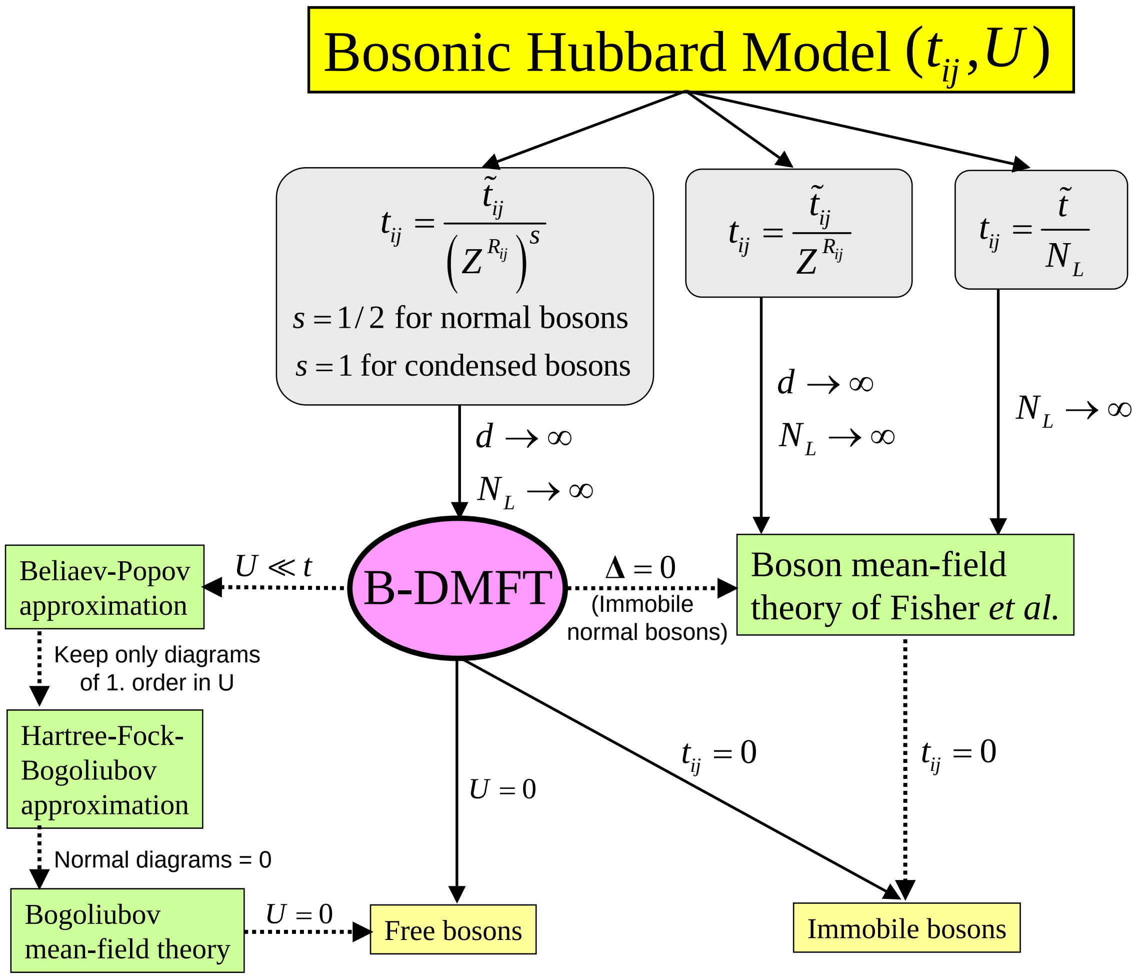
$$\kappa \int_0^\beta d\tau \bar{\phi}^\dagger(\tau)\bar{b}(\tau) + \frac{U}{2}\int_0^\beta n(\tau)(n(\tau) - 1)$$

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

(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 Generalized Gross-Pitaevskii equation

Condensate wave function

$$\Phi(\tau) = \langle b(\tau) \rangle_{S_{loc}} \Longleftrightarrow \langle \delta S_{loc} / \delta b^* \rangle_{S_{loc}} = 0$$

Approximation: $b(\tau) \to \langle b(\tau) \rangle_{S_{loc}} \equiv \Phi(\tau)$

$$\frac{\partial \Phi(\tau)}{\partial \tau} = \left[\mu - \kappa - U |\Phi(\tau)|^2 \right] \Phi(\tau) + \int_0^\beta d\tau' \left[\Delta^{11}(\tau - \tau')\Phi(\tau') + \Delta^{12}(\tau - \tau')\Phi^*(\tau') \right]$$

Generalized Gross-Pitaevski equation includes retardation effects due to normal bosons

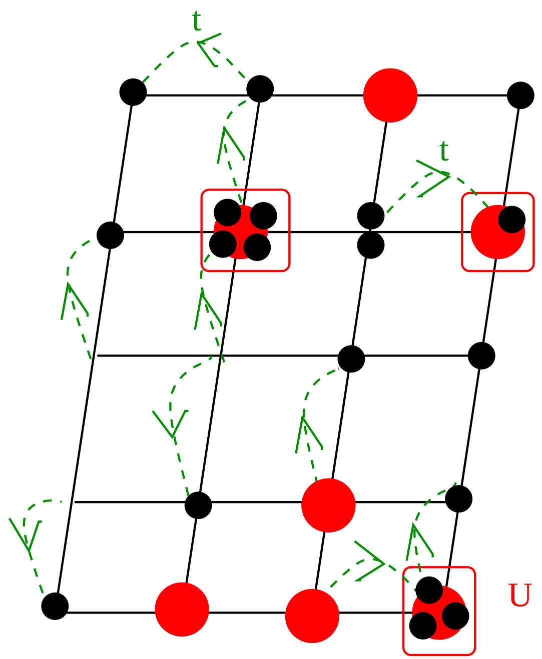
B-DMFT application to bosonic Falicov-Kimball model

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

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

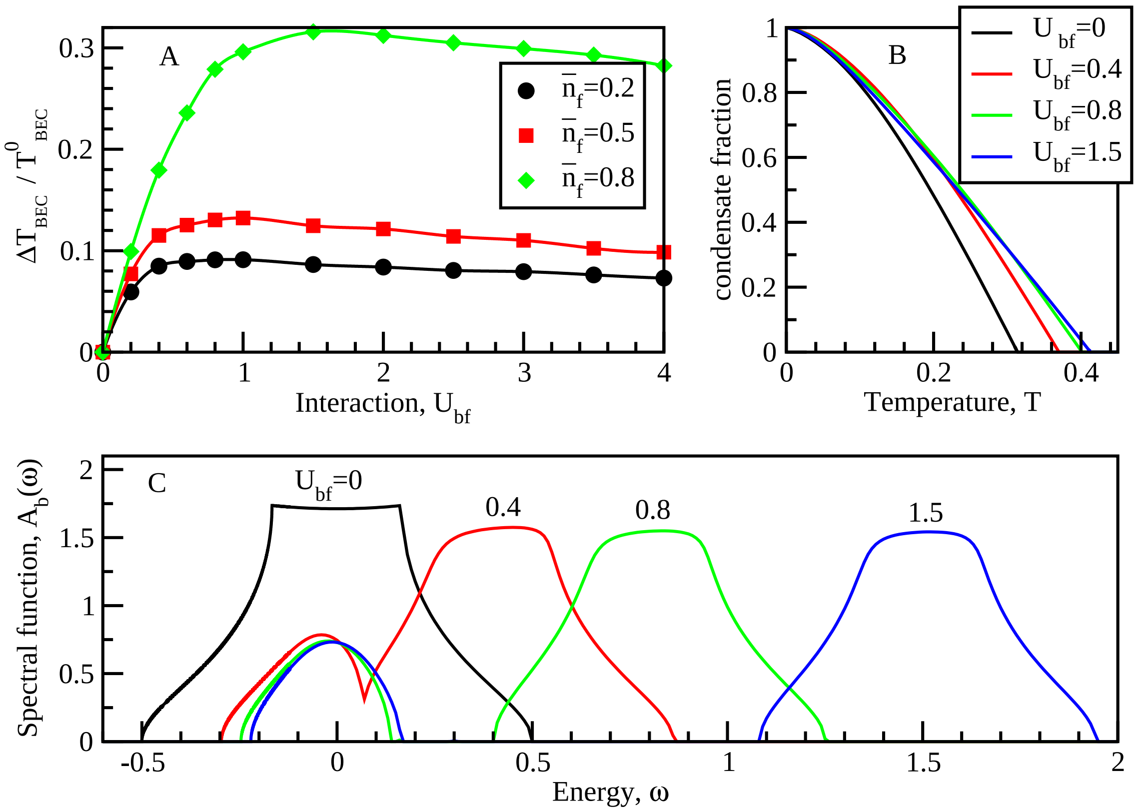
Local conservation law $[n_{fi}, H] = 0$ hence $n_{fi} = 0, 1, 2, \ldots$ classical variable

B-DMFT: local action Gaussian and analytically integrable



Enhancement of T_{BEC} due to interaction

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



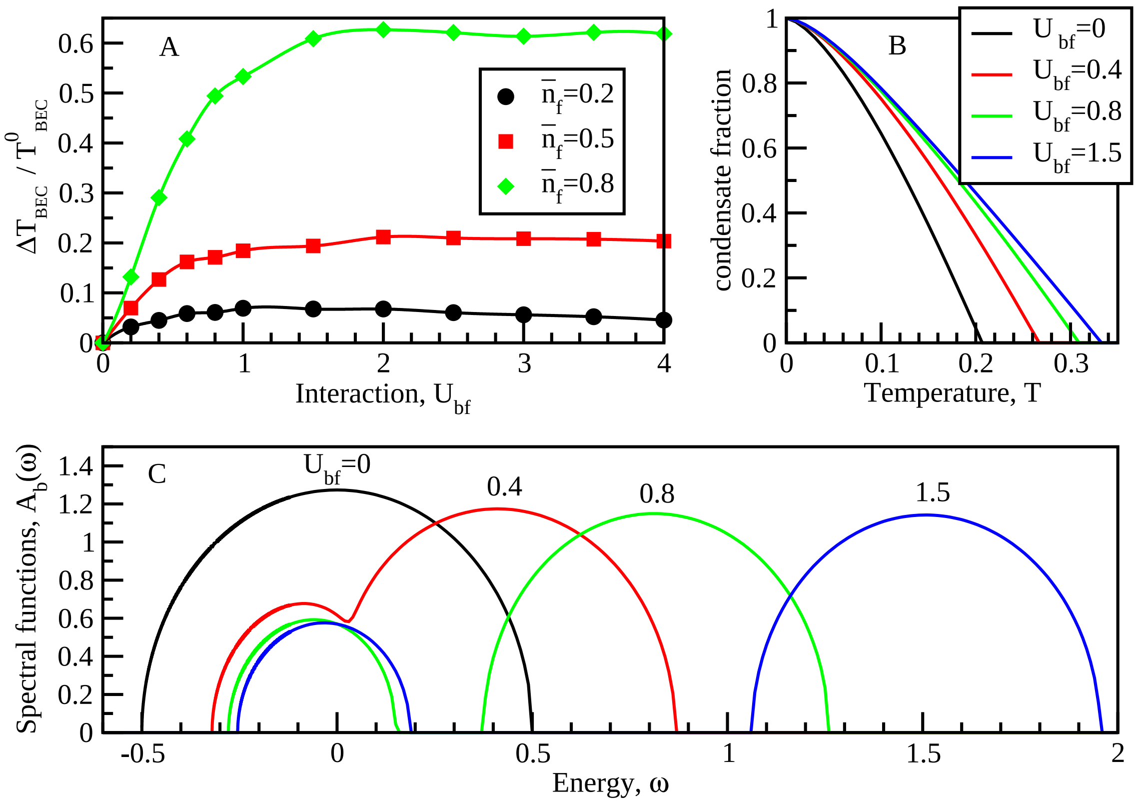
$$A_b(\omega) = -\mathrm{Im}G_b(\omega)/\pi$$

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

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



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

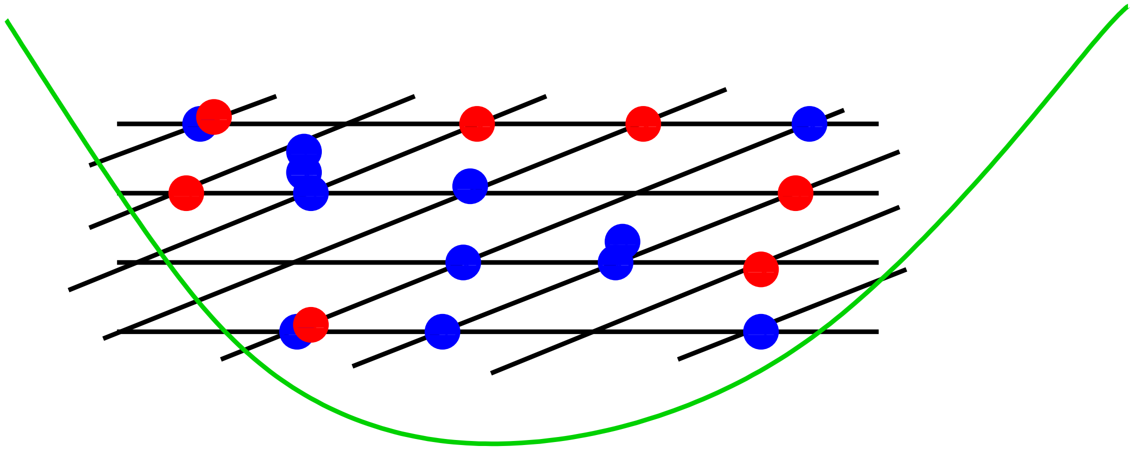
$$\bar{n}_b = \bar{n}_b^{BEC} + \int d\omega \, \frac{A_b(\omega+\mu_b)}{e^{\omega/T}-1}$$

Normal part decreases when U increases for constant μ_b and T

BOSONS and FERMIONS

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:

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

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

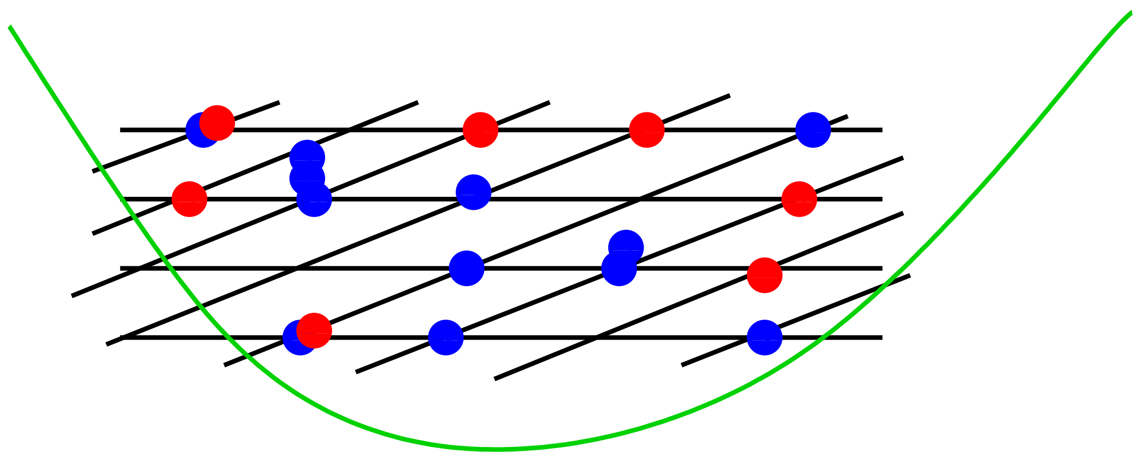
$$S_{i_0}^{\mathrm{f}} = \int_0^\beta d\tau f_{i_0}^*(\tau) \left(\partial_\tau - \mu_f + \epsilon_{i_0}^f\right) f_{i_0}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' f_{i_0}^*(\tau) \Delta_{i_0}^f(\tau - \tau') f_{i_0}(\tau')$$

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

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

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

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

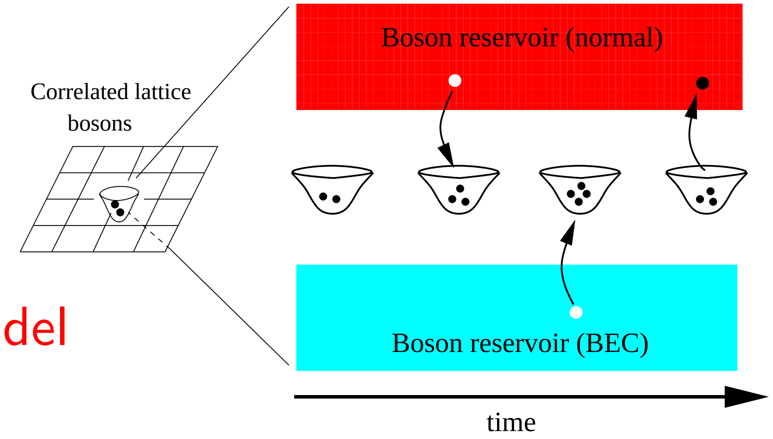
Boson-Boson interaction

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

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!