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


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

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

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:

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

\[ \frac{1}{N_L} E_{\text{kin}} = \frac{1}{N_L} \sum_{ij\sigma} t_{ij} \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle = \infty ! \]

Overscaling fermions

\[ t_{ij} = \frac{t_{ij}^*}{d||R_i - R_j||}, \quad U = U, \quad \text{etc.} \]

\[ \frac{1}{N_L} E_{\text{kin}} = \frac{1}{N_L} \sum_{ij\sigma} t_{ij} \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle = 0 ! \]
Fermions in large dimensions (coordination)

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

\[
\frac{1}{N_L} E_{\text{kin}} = \frac{1}{N_L} \sum_{i,j,\sigma} t_{ij} \langle c^\dagger_{i\sigma} c_{j\sigma} \rangle = \frac{1}{N_L} \sum_{i,\sigma} \sum_{j(i)} t_{ij} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} G_{ij\sigma}(\omega) \sim O(1)
\]

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

\[
G_{ij} \sim O(d^{-\frac{||R_i-R_j||}{2}})
\]

with rescaling

\[
t_{ij} \rightarrow \frac{t_{ij}^*}{\sqrt{d||R_i-R_j||}}
\]

sum \( \sum_{j(i)} \) is compensated and energy is finite (Metzner, Vollhardt, 1989)
Comprehensive mean-field theory for fermions

\[ H = H^{\text{hopping}} + H^{\text{interaction}}_{\text{loc}} \]

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

\[ \langle H \rangle, \quad \langle H^{\text{hopping}} \rangle, \quad \langle H^{\text{interaction}}_{\text{loc}} \rangle \]

are finite and generically non-zero, and

\[ \langle [H^{\text{hopping}}, H^{\text{interaction}}_{\text{loc}}] \rangle \neq 0 \]

to describe non-trivial competition
Non-comprehensive mean-field theory for fermions

- Distance independent hopping (van Dongen, Vollhardt 92)

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

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

\[ H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{i,j} n_{i\uparrow} n_{j\downarrow} = \sum_{k,\sigma} \epsilon_k n_{k\sigma} + U \sum_k n_{k\uparrow} n_{k\downarrow} \]

In both models a non-trivial competition is suppressed

\[ \langle [H^{\text{hopping}}, H^{\text{interaction}}] \rangle = 0 \]

although \( \langle H \rangle, \langle H^{\text{hopping}} \rangle, \langle H^{\text{interaction}} \rangle \neq 0 \)
\( d \to \infty \) limit – Feynman diagrams simplification

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

\[
\Sigma_{ij\sigma}(\omega_n) \to_{d \to \infty} \Sigma_{i\sigma}(\omega_n) \delta_{ij}
\]

Fourier transform is \( k \)-independent

\[
\Sigma(\mathbf{k}, \omega_n) \to_{d \to \infty} \Sigma(\omega_n)
\]

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

\[ S_{loc} = -\sum_\sigma \int d\tau d\tau' c_\sigma^*(\tau)G_\sigma^{-1}(\tau - \tau')c_\sigma(\tau') + U \int d\tau n_\uparrow(\tau)n_\downarrow(\tau) \]

Weiss (mean-field) function and self-energy

\[ G_\sigma^{-1}(\omega_n) = G_\sigma^{-1}(\omega_n) + \Sigma_\sigma(\omega_n) \]

Local Green function and lattice system self-consistency

\[ G_\sigma(i\omega_n) = \sum_k G_\sigma(k, \omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_\sigma(\omega_n)} = G_\sigma^0(i\omega + \mu - \Sigma_\sigma(\omega_n)) \]
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

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

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

$\hat{H}^0$ is a model TB or a microscopic LDA Hamiltonian
BOSONS
Correlated bosons on optical lattices

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

\[ E_{\text{int}} = U \]

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

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

Not sufficient for bosons because of BEC:

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

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

- 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:
  \[ \frac{1}{N_L} E_{\text{kin}} = \infty \]

- Fractional scaling:
  \[ \frac{1}{N_L} E_{\text{kin}} = \infty \]
  in the BEC phase

- Integer scaling:
  \[ \frac{1}{N_L} E_{\text{kin}} = 0 \]
  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: $t_{ij} = \frac{t_{ij}^*}{(2d)^{\frac{d-2}{2}} ||R_i - R_j||}$ - fractional rescaling

   - BEC parts: $t_{ij} = \frac{t_{ij}^*}{(2d)^{\frac{d-2}{2}} ||R_i - R_j||}$ - 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 $d \to \infty$)

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

(ii) Local impurity  

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

\[
S_{loc} = -\int_0^\beta \int_0^\beta d\tau d\tau' \hat{b}^\dagger(\tau) \hat{G}^{-1}(\tau - \tau') \hat{b}(\tau) + \kappa \int_0^\beta d\tau \bar{\phi}^\dagger(\tau) \bar{b}(\tau) + \frac{U}{2} \int_0^\beta n(\tau) (n(\tau) - 1)
\]

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

(iii) Condensate wave function

\[
\bar{\phi}(\tau) = \int D[b^*, b] \bar{b}(\tau) e^{-S_{loc}}
\]
B-DMFT in well-known limits

Bosonic Hubbard Model \((t_{ij}, U)\)

- \(t_{ij} = \frac{t_{ij}}{(Z_{R_i}^s)^s}\)
  - \(s = \frac{1}{2}\) for normal bosons
  - \(s = 1\) for condensed bosons
- \(d \to \infty\)
- \(N_L \to \infty\)

Boson mean-field theory of Fisher et al.

- \(d \to \infty\)
- \(N_L \to \infty\)

Beliaev-Popov approximation

- \(U \ll t\)
- Keep only diagrams of 1. order in \(U\)

Hartree-Fock-Bogoliubov approximation

- Normal diagrams = 0

Bogoliubov mean-field theory

- \(U = 0\)

Free bosons

Immobile bosons

B-DMFT

- \(\Lambda = 0\)
- (Immobile normal bosons)
- \(t_{ij} = 0\)

Keep only diagrams of 1. order in \(U\)
**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

\begin{align*}
A_b(\omega) &= -\text{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}
\end{align*}

Normal part decreases when $U$ increases for constant $\mu_b$ 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

\[ A_b(\omega) = -\text{Im}G_b(\omega)/\pi \]

\[ \bar{n}_b = \bar{n}_{b}^{BEC} + \int d\omega \frac{A_b(\omega + \mu_b)}{e^{\omega/T} - 1} \]

Normal part decreases when $U$ increases for constant $\mu_b$ and $T$
Bose-Fermi mixtures ($^{87}$Rb-$^{40}$K) on a lattice with a trap

$$H = \sum_{ij} t_{ij}^b b_i^\dagger b_j + \sum_i \epsilon_i^b n_i^b + \frac{U_b}{2} \sum_i n_i^b (n_i^b - 1) + \sum_{ij} t_{ij}^f f_i^\dagger f_j + \sum_i \epsilon_i^f n_i^f + U_{bf} \sum_i n_i^b n_i^f$$
DMFT for bose-fermi mixtures

BF-DMFT equations:

\[
S^{b}_{i0} = \int_{0}^{\beta} d\tau b^\dagger_{i0}(\tau) \left( \partial_{\tau} \sigma_3 - (\mu_b - \epsilon_{i0}^b) 1 \right) b_{i0}(\tau) + \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' b^\dagger_{i0}(\tau) \Delta_{i0}^b(\tau - \tau') b_{i0}(\tau')
\]

\[
+ \frac{U_b}{2} \int_{0}^{\beta} n_{i0}^b(\tau)(n_{i0}^b(\tau) - 1) + \int_{0}^{\beta} d\tau \sum_{j \neq i0} t_{i0j}^b b^\dagger_{i0}(\tau) \Phi_j(\tau)
\]

\[
S^{f}_{i0} = \int_{0}^{\beta} d\tau f^*_{i0}(\tau) \left( \partial_{\tau} - \mu_f + \epsilon_{i0}^f \right) f_{i0}(\tau) + \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' f^*_{i0}(\tau) \Delta_{i0}^f(\tau - \tau') f_{i0}(\tau')
\]

\[
S^{bf}_{i0} = U_{bf} \int_{0}^{\beta} d\tau n_{i0}^b(\tau) n_{i0}^f(\tau)
\]
Lattice self-consistency (Dyson) equations

\[ G^{b}_{ij}(i\nu_n) = \left[ (i\nu_n\sigma_3 + \mu_b 1 - \Sigma^{b}_i(i\nu_n))\delta_{ij} - t^{b}_{ij} 1 \right]^{-1} \]

\[ G^{f}_{ij}(i\omega_n) = \left[ (i\omega_n + \mu_f - \Sigma^{f}_i(i\omega_n))\delta_{ij} - t^{f}_{ij} \right]^{-1} \]
Integrating out fermions

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

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

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

\[ \ln \det [M^b] = \text{Tr} \ln [M^b] = \text{Tr} \ln [-(G^f)^{-1} + M_1^b] = \text{Tr} \ln [-(G^f)^{-1}] - \sum_{m=1}^{\infty} \frac{1}{m} \text{Tr} [G^f M_1^b]^m \]

\[ G^f_{i_0}(\omega_n) = \frac{1}{i \omega_n + \mu_f - \epsilon^f_{i_0} - \Delta^f_{i_0}(\omega_n)} \]

Effective bosonic action

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

\[ \pi^f_{i_0}(\nu_n) = -\frac{1}{\beta} \sum_m G^f_{i_0}(\omega_m) G^f_{i_0}(\omega_m + \nu_n) \]

Boson-Boson interaction

\[ U_{b}^{\text{eff}} = U_b - U_{bf}^2 N^f_{i_0}(\mu) \]

System unstable when \( U_b = U_{bf}^2 N^f_{i_0}(\mu) \).
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!