Bose-Hubbard model and Bose-Einstein condensation on infinite-dimensional lattice

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New results

- New way of rescaling hopping to obtain non-trivial $d \to \infty$ limt including BEC condensate and normal bosons

- New DMFT equations for Bose-Hubbard model

$$S_{imp} = \int_0^\beta \int_0^\beta d\tau d\tau' \bar{b}^\dagger(\tau) \, \widehat{\mathcal{G}}^{-1}(\tau - \tau') \, \bar{b}(\tau) - 2t^* \int_0^\beta d\tau \bar{\phi}^\dagger(\tau) \bar{b}(\tau) + \frac{U}{2} \int_0^\beta n(\tau)(n(\tau) - 1)$$

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

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

$$\partial_\tau \bar{\phi}(\tau) - \int_0^\beta d\tau' \widehat{\Delta}(\tau - \tau') \bar{\phi}(\tau') - 2t^* \bar{\phi}(\tau) + U |\bar{\phi}(\tau)|^2 \bar{\phi}(\tau) = \mu \bar{\phi}(\tau)$$

Outline

1. Non-text book remarks on Bose-Einstein Condensation (BEC)

2. Bose-Hubbard model on the lattice and $d \to \infty$ limit

3. Cavity method and DMFT equations

4. Discussion and conclusions

Support from SFB 484

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 taką 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: types of BEC

H.B.G. Casimir 1968 - notes that the distribution strongly depends on the boundary condition; three different types of BEC:

- Type I: single state macroscopically occupied

$$\lim_{V\to\infty} \frac{n_0}{V} = O(1),$$

  others $O(1/V)$

- Type II: infinite states in a band B_V macroscopically occupied

$$\lim_{V\to\infty} \frac{n_k}{V} = O(1),$$

  where $k \in B_V$, others $O(1/V)$

- Type III: (non-extensive occupation) none state macroscopically occupied but

$$\lim_{V\to\infty} \sum_{k\in B_V} \frac{n_k}{V} = O(1),$$

  others $O(1/V)$, c.f. Physica **110A**, 550 (1982).

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 $n_0 = N_c \sim O(N)$

BEC and ODLRO on the lattice

Wannier representation $\psi(r) = \sum_i b_i w_i(r)$, where $[b_i, b_j^\dagger] = \delta_{ij}$,

$$H = \sum_{ij} t_{ij} b_i^\dagger b_j$$

one-particle density matrix is Hermitian $\rho_{ij}^* = \rho_{ji}$

$$\rho_{ij} = \rho(R_i, R_j) = \langle b_i^\dagger b_j \rangle = \underbrace{N_c \chi_0^*(R_i)\chi_0(R_j)}_{\text{BEC}} + \underbrace{\sum_{\alpha \neq 0} n_\alpha \chi_\alpha^*(R_i)\chi_\alpha(R_j)}_{\text{normal part}}$$

Lattice Fourier transform: $\chi_k(R_i) = \frac{1}{\sqrt{N_L}} e^{ikR_i}$, $b_i = \frac{1}{\sqrt{N_L}} \sum_k e^{-ikR_i} b_k$, $n_k = \langle b_k^\dagger b_k \rangle$

$$\rho_{ij} = \frac{1}{N_L} \sum_k n_k e^{ik(R_i - R_j)} = \underbrace{\frac{N_c}{N_L}}_{\text{BEC}} + \underbrace{\frac{1}{N_L} \sum_{k \neq 0} n_k e^{ik(R_i - R_j)}}_{\text{normal part}}$$

BEC and ODLRO on the lattice

$$\rho_{ij} = \underbrace{\frac{N_c}{N_L}}_{\text{BEC part}} + \underbrace{\frac{1}{N_L}\sum_{k\neq 0} n_k e^{ik(R_i-R_j)}}_{\text{normal part}} \underbrace{\longrightarrow}_{|R_i-R_j|\to\infty} \frac{N_c}{N_L} = n_c$$

- BEC part exhibilts long-range order, does not depend on $|R_i - R_j|$
- normal part vanishes due to destructive interference between different waves

in the presence of BEC both contributions to the density matrix
behave differently with respect to $|R_i - R_j|$

BEC on the lattice in $d \to \infty$ limit

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

- quantum $t_{ij} = \frac{t^*_{ij}}{(2d)^{\frac{||R_i - R_j||}{2}}}$ leads to finite kinetic energy $E_{\rm kin}$ when $d \to \infty$
- classical $t_{ij} = \frac{t^*_{ij}}{d^{||R_i - R_j||}}$ leads to $E_{\rm kin} \to 0$ when $d \to \infty$
- nothing $t_{ij} = t^*_{ij}$ leads to $E_{\rm kin} \to \infty$ when $d \to \infty$

Check bosons:

$$E_{\rm kin} = \sum_{ij} t_{ij}\rho_{ij} = \sum_{i=1}^{N_L} \underbrace{\sum_{j}^{2d}}_{\sim d} \overbrace{t^{nn}_{ij}}^{t^{nn} = \frac{t^*}{d}} \underbrace{\frac{N_c}{N_L}}_{\rm ODLRO} + \ldots + \frac{1}{N_L} \sum_{i}^{N_L} \underbrace{\sum_{j}^{2d}}_{\sim 2d} \overbrace{t^{nn}_{ij}}^{t^{nn} = \frac{t^*}{\sqrt{2d}}} \underbrace{\sum_{k \neq 0} n_k e^{ik(R_i - R_j)}}_{\sim \frac{1}{\sqrt{2d}}} + \ldots$$

$\Longrightarrow$ Two different rescaling are needed when BEC is present

BEC on the lattice in $d \to \infty$ limit

We propose:

1. rescaling is made inside an effective potential (energy, action, Lagrangian, Hamiltonian, etc.) but not at the level of a bare Hamiltonian operator

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

2. limit $d \to \infty$ taken afterwards in this effective potential

such procedure gives consistent derivation of DMFT equations as exact ones in $d \to \infty$ limit for boson models with local interactions

Bose-Hubbard model

Bose-Hubbard Hamiltonian

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

partition function

$$Z = \int \prod_i D[b_i^*, b_i] e^{-S[b_i^*, b_i]}$$

averages

$$\langle \hat{A} \rangle = \frac{\int \prod_i D[b_i^*, b_i] A[b_i^*, b_i] e^{-S[b_i^*, b_i]}}{\int \prod_i D[b_i^*, b_i] e^{-S[b_i^*, b_i]}}$$

action

$$S[b_i^*, b_i] = \int_0^\beta d\tau \left(\sum_i b_i^*(\tau)(\partial_\tau - \mu) b_i(\tau) - \sum_{ij} t_{ij} b_i^*(\tau) b_j(\tau) + \frac{U}{2} \sum_i n_i(\tau)[n_i(\tau) - 1] \right)$$

Bose-Hubbard model in $d \to \infty$ limit

A. Georges and G. Kotliar 1992 - cavity method, integrate out all sites $i \neq 0$

$$Z = \int D[b_0^*, b_0] e^{-S_0[b_0^*, b_0]} \int \prod_{i \neq 0} D[b_i^*, b_i] e^{-S^{[0]}[b_i^*, b_i]} \underbrace{e^{-\Delta S[b_i^*, b_i, b_0^*, b_0]}}_{\text{cummulant expansion}}$$

$$S_0[b_0^*, b_0] = \int_0^\beta d\tau \left(b_0^*(\tau)(\partial_\tau - \mu) b_0(\tau) + \frac{U}{2} n_0(\tau)[n_0(\tau) - 1] \right)$$

$$S^{[0]}[b_i^*, b_i] = \int_0^\beta d\tau \left(\sum_{i \neq 0} b_i^*(\tau)(\partial_\tau - \mu) b_i(\tau) - \sum_{ij \neq 0} t_{ij} b_i^*(\tau) b_j(\tau) + \frac{U}{2} \sum_{i \neq 0} n_i(\tau)[n_i(\tau) - 1] \right)$$

$$\Delta S[b_i^*, b_i, b_0^*, b_0] = -\int_0^\beta d\tau \sum_{i \neq 0} [t_{i0} b_i^*(\tau) b_0(\tau) + t_{0i} b_0^*(\tau) b_i(\tau)] \equiv \int_0^\beta d\tau \Delta S(\tau)$$

Bose-Hubbard model in $d \to \infty$ limit

$$Z = \int D[b_0^*, b_0] e^{-S_0[b_0^*, b_0]} Z_{S^{[0]}} [1 - \int_0^\beta d\tau \langle \Delta S(\tau) \rangle_{S^{[0]}}^{\text{dis}} + \frac{1}{2!} \int_0^\beta d\tau_1 d\tau_2 \langle \Delta S(\tau_1) \Delta S(\tau_2) \rangle_{S^{[0]}}^{\text{dis}} + \ldots]$$

$$Z_{S^{[0]}} = \int \prod_{i \neq 0} D[b_i^*, b_i] e^{-S^{[0]}[b_i^*, b_i]}$$

$$\frac{Z}{Z_{S^{[0]}}} = \int D[b_0^*, b_0] e^{-S_{\text{eff}}[b_0^*, b_0]}$$

$$S_{\text{eff}}[b_0^*, b_0] = \int_0^\beta d\tau \left(b_0^*(\tau)(\partial_\tau - \mu) b_0(\tau) + \frac{U}{2} n_0(\tau)[n_0(\tau) - 1] \right) +$$

$$\sum_{n=1}^{\infty} \sum_{i_1 \ldots j_n} \int d\tau_{i_1} \ldots d\tau_{j_n} b_0^{(*)}(\tau_{i_1}) \ldots b_0^{(*)}(\tau_{j_n}) t_{i_1 0} \ldots t_{0 j_n} \hat{G}_{i_1 \ldots j_n}^{[0]\text{con}}(\tau_{i_1} \ldots \tau_{j_n})$$

Theorem

In $d \to \infty$ limit when new rescaling applied only terms with $n = 1$ and 2 appear

Bose-Hubbard model in $d \to \infty$ limit

$n = 1$ term $\langle \Delta S(\tau) \rangle$:

$$\sim \underbrace{\sum_{i(0)}}_{\sim d} \int_0^\beta d\tau \underbrace{t_{i0}}_{t=\frac{t^*}{d} \text{ classical rescalling}} \underbrace{\overbrace{\langle b_i^*(\tau) \rangle_{S^{[0]}}}^{\equiv \phi_i(\tau) \text{ order parameter, connected}}}_{\text{ODLRO}} b_0(\tau) + h.c. \quad [\sim O(1)]$$

$n = 2$ term $\langle \Delta S(\tau) \Delta S(\tau') \rangle$, e.g. $i \neq j$:

$$\sim \sum_{ij(0)} t_{i0} t_{0j} \bar{b}_0(\tau)^\dagger \hat{G}_{ij}^{[0]\text{dis}}(\tau - \tau') \bar{b}_0(\tau') = \underbrace{\sum_{ij(0)}}_{\sim d^2} \underbrace{t_{i0} t_{0j}}_{\frac{t^*}{\sqrt{d}} \frac{t^*}{\sqrt{d}}} \bar{b}_0^\dagger(\tau) \underbrace{\hat{\tilde{G}}_{ij}^{[0]\text{con}}(\tau - \tau')}_{\frac{1}{\left(\sqrt{d}\right)^2}} \bar{b}_0(\tau') + \quad [\sim O(1)]$$

$$+ \underbrace{\sum_{ij(0)}}_{\sim d^2} \underbrace{t_{i0} t_{0j}}_{\frac{t^*}{d} \frac{t^*}{d}} \bar{b}_0^\dagger(\tau) \underbrace{\overbrace{\Phi_i^\dagger(\tau) \Phi_j(\tau')}^{\text{disconnected}}}_{ODLRO} \bar{b}_0(\tau') \quad [\sim O(1)]$$

where $\bar{b} = (b, b^*)$, $\Phi = (\phi, \phi^*)$, $\hat{\tilde{G}} = \begin{pmatrix} \tilde{G}_{11} & \tilde{G}_{12} \\ \tilde{G}_{21} & \tilde{G}_{22} \end{pmatrix}$ and $\hat{G}^{\text{dis}} = \hat{\tilde{G}}^{\text{con}} + \Phi^* \Phi$

Bose-Hubbard model in $d \to \infty$ limit

$n = 3$ term $\langle \Delta S(\tau) \Delta S(\tau') \Delta S(\tau'') \rangle$, e.g. $i \neq j \neq k$:

$$\sim \underbrace{\sum_{ijk(0)}}_{\sim d^3} \underbrace{t_{i0} t_{j0} t_{k0}}_{\frac{t^*}{d}\frac{t^*}{d}\frac{t^*}{d}} \overbrace{\underbrace{\Phi_i(\tau)\Phi_j(\tau')\Phi_k(\tau'')}_{\text{ODLRO}}}^{\text{disconnected}} \bigotimes \bar{b}_0(\tau)\bar{b}_0(\tau')\bar{b}_0(\tau'') + \quad [\sim \; O(1)]$$

$$\underbrace{\sum_{ijk(0)}}_{\sim d^3} \underbrace{t_{i0} t_{j0} t_{k0}}_{\frac{t^*}{d}\frac{t^*}{\sqrt{d}}\frac{t^*}{\sqrt{d}}} \overbrace{\underbrace{\Phi_i(\tau)}_{\text{ODLRO}} \; \underbrace{\hat{\tilde{G}}^{[0]\text{con}}_{jk}(\tau' - \tau'')}_{\frac{1}{(\sqrt{d})^2}}}^{\text{disconnected}} \bigotimes \bar{b}_0(\tau)\bar{b}_0(\tau')\bar{b}_0(\tau'') + \quad [\sim \; O(1)]$$

$$\underbrace{\sum_{ijk(0)}}_{\sim d^3} \underbrace{t_{i0} t_{j0} t_{k0}}_{\frac{t^*}{\sqrt{d}}\frac{t^*}{\sqrt{d}}\frac{t^*}{\sqrt{d}}} \underbrace{\hat{\tilde{G}}^{[0]\text{con}}_{ijk}(\tau, \tau', \tau'')}_{\frac{1}{(\sqrt{d})^4}} \bigotimes \bar{b}_0(\tau)\bar{b}_0(\tau')\bar{b}_0(\tau'') \qquad [\sim \; O\left(\frac{1}{\sqrt{d}}\right)]$$

and for each n separately ...

Bose-Hubbard model in $d \to \infty$ limit, DMFT

Effective local action:

$$S_{imp} = \int_0^\beta \int_0^\beta d\tau d\tau' \bar{b}^\dagger(\tau)\, \widehat{\mathcal{G}}^{-1}(\tau - \tau')\, \bar{b}(\tau) - 2t^* \int_0^\beta d\tau \bar{\phi}^\dagger(\tau)\bar{b}(\tau) + \frac{U}{2} \int_0^\beta n(\tau)(n(\tau) - 1)$$

where

$$\hat{\mathcal{G}}^{-1}(\tau - \tau') = \delta(\tau - \tau') \begin{pmatrix} \partial_\tau - \mu & 0 \\ 0 & \partial_\tau - \mu \end{pmatrix} + \frac{1}{2} \sum_{i,j \neq 0} t^*_{i0} t^*_{j0} \hat{\hat{G}}^{[0]\text{con}}_{ij}(\tau - \tau')$$

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

k-integrated Dyson equation

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

Bose-Hubbard model, DMFT and Gross-Pitaevskii equation

classical (ODLRO) $\bar{\phi}(\tau)$ fields not yet determined
use classical Euler-Lagrange equations with translaional invariance

$$\frac{\delta S_{\rm imp}[b_0, b_0^*]}{\delta b_0(\tau)}|_{\bar{b}_0(\tau)=\bar{\phi}(\tau)} = 0$$

Gross-Pitaevskii equations for DMFT

$$\partial_\tau \bar{\phi}(\tau) - \int_0^\beta d\tau' \widehat{\Delta}(\tau - \tau')\bar{\phi}(\tau') - 2t^* \bar{\phi}(\tau) + U|\bar{\phi}(\tau)|^2 \bar{\phi}(\tau) = \mu \bar{\phi}(\tau)$$

DMFT equations for Bose-Hubbard model

i) Action

$$S_{imp} = \int_0^\beta \int_0^\beta d\tau d\tau' \bar{b}^\dagger(\tau)\, \widehat{\mathcal{G}}^{-1}(\tau - \tau')\, \bar{b}(\tau) - 2t^* \int_0^\beta d\tau \bar{\phi}^\dagger(\tau)\bar{b}(\tau) + \frac{U}{2} \int_0^\beta n(\tau)(n(\tau) - 1)$$

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

ii) Integrated Dyson (lattice self-consistency) equation

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

iii) Generalized Gross-Pitaevskii equation

$$\partial_\tau \bar{\phi}(\tau) - \int_0^\beta d\tau' \widehat{\Delta}(\tau - \tau')\bar{\phi}(\tau') - 2t^* \bar{\phi}(\tau) + U|\bar{\phi}(\tau)|^2 \bar{\phi}(\tau) = \mu \bar{\phi}(\tau)$$

Outlook

- checked - all known limits (Bogoliubov, Hartree-Fock-Bogoliubov, Popov) satisfied

- obtained theory: consistent, conserving, exact in d or $z \to \infty$ limit, valid for all U, T, n, arbitrary lattice (tree) $\Longrightarrow$ the mean-field theory

- useful impurity solver (???): should satisfy Hugenholtz-Pines theorem 1959 - gapless spectrum in BEC phase, i.e.

$$\mu = \Sigma_{11}(\omega = 0) - \Sigma_{12}(\omega = 0)$$

- Hamiltonian representation: generalized single impurity Anderson model with nonconserving particle number

- many things to do .... collaboration wanted