Developing the bosonic DMFT formalism

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Phys. Rev. Lett. **105**, 096402 (2010)

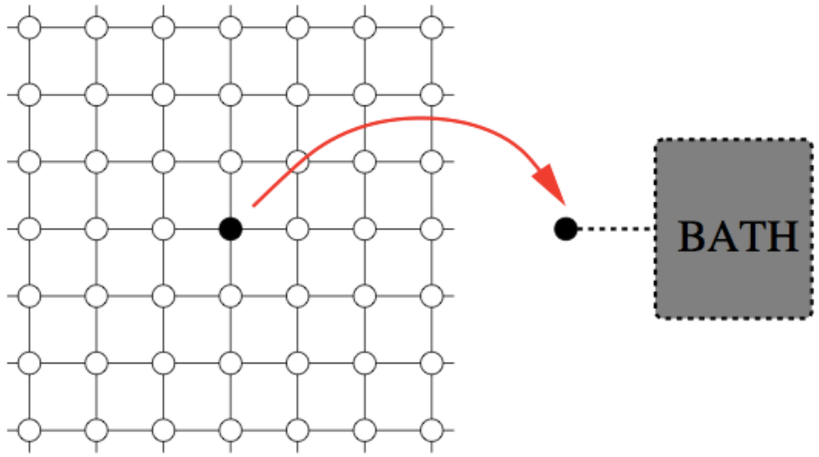
previous approaches : Byczuk/Vollhardt, Hubener/Snoek/Hofstetter, Hu/Tong, F. Zamponi *et al.*

Outline

- Introduction
  - DMFT in a nutshell
  - DMFT in cold cases
- Developing the Bose DMFT formalism (BDMFT)
  - weakly interacting Bose gas physics
  - BDMFT action
  - effective medium approach
  - cavity method
  - kinetic energy functional approximation
- Results
- Conclusions and Outlook

mean-field theory

A. Georges, Lectures on the Physics of Highly Correlated Electron Systems VIII (2004) 3, American Institute of Physics Conference Proceedings Vol. 715, arXiv:0403123 (2004).



classical Ising (ferromagnet J > 0):

$$H = -J \sum_{\langle i,j \rangle} S_i S_j + h \sum_i S_i$$

we are interested in the magnetization on every site:

$$m_i = \langle S_i \rangle$$

Weiss field:

$$H_{\text{eff}} = -\sum_i h_i^{\text{eff}} S_i \qquad \beta h_i^{\text{eff}} = \tanh^{-1} m_i$$

approximation:

$$h_i^{\text{eff}} \approx h + \sum_j J m_j = h + zJm$$

selfconsistency equation :

$$m = \tanh(\beta h + z\beta J m)$$

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A. Georges, Lectures on the Physics of Highly Correlated Electron Systems VIII (2004) 3, American Institute of Physics Conference Proceedings Vol. 715, arXiv:0403123 (2004).

Consider the Hubbard model for fermions:

$$H = -\sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \varepsilon_0 \sum_{i\sigma} n_{i\sigma}$$

The full Green function can be written as:

$$G(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \varepsilon_0 - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, i\omega_n)} \qquad \varepsilon_{\mathbf{k}} \equiv \sum_j t_{ij} e^{i\mathbf{k}.(\mathbf{R}_i - \mathbf{R}_j)}$$

We are interested in the local Green function, but with time dependence:

$$G^{\sigma}_{ii}(\tau - \tau') \equiv -\langle T c_{i\sigma}(\tau) c^{\dagger}_{i\sigma}(\tau') \rangle$$

Analogous to mean-field theory, we map onto an Anderson impurity model

$$H_{AIM} = H_{atom} + H_{bath} + H_{coupling}$$

$$H_{atom} = U\, n^c_{\uparrow} n^c_{\downarrow} + (\varepsilon_0 - \mu)\,(n^c_{\uparrow} + n^c_{\downarrow})$$

$$H_{bath} = \sum_{l\sigma} \tilde{\varepsilon}_l\, a^{\dagger}_{l\sigma} a_{l\sigma}$$

$$H_{coupling} = \sum_{l\sigma} V_l\, (a^{\dagger}_{l\sigma} c_{\sigma} + c^{\dagger}_{\sigma} a_{l\sigma})$$

The effective parameters enter only through the hybridization function:

$$\Delta(i\omega_n) = \sum_l \frac{|V_l|^2}{i\omega_n - \tilde{\varepsilon}_l}$$

DMFT 101

A. Georges, Lectures on the Physics of Highly Correlated Electron Systems VIII (2004) 3, American Institute of Physics Conference Proceedings Vol. 715, arXiv:0403123 (2004).

Rewrite by integrating out the bath degrees of freedom :

$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^+(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_\sigma(\tau') + U\int_0^\beta d\tau\, n_\uparrow(\tau)n_\downarrow(\tau)$$

with: $\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \varepsilon_0 - \Delta(i\omega_n)$

The impurity selfenergy can be calculated by solving the impurity problem:

$$\begin{aligned}\Sigma_{imp}(i\omega_n) \equiv & \quad \mathcal{G}_0^{-1}(i\omega_n) - G^{-1}(i\omega_n) \\ = & \quad i\omega_n + \mu - \varepsilon_0 - \Delta(i\omega_n) - G^{-1}(i\omega_n)\end{aligned}$$

Now comes the approximation in which we neglect all non-local components of the selfenergy: $\Sigma_{ii} \simeq \Sigma_{imp}\ ,\ \Sigma_{i\neq j} \simeq 0$

The selfconsistency requirement is then: $$\sum_{\mathbf{k}} \frac{1}{\Delta(i\omega_n) + G(i\omega_n)^{-1} - \varepsilon_{\mathbf{k}}} = G(i\omega_n)$$

or, using the density of states, $D(\varepsilon) \equiv \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}})$

$$\int d\varepsilon \frac{D(\varepsilon)}{\Delta(i\omega_n) + G(i\omega_n)^{-1} - \varepsilon} = G(i\omega_n)$$

DMFT 101

A. Georges, Lectures on the Physics of Highly Correlated Electron Systems VIII (2004) 3, American Institute of Physics Conference Proceedings Vol. 715, arXiv:0403123 (2004).

$$H = -\sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \varepsilon_0 \sum_{i\sigma} n_{i\sigma}$$

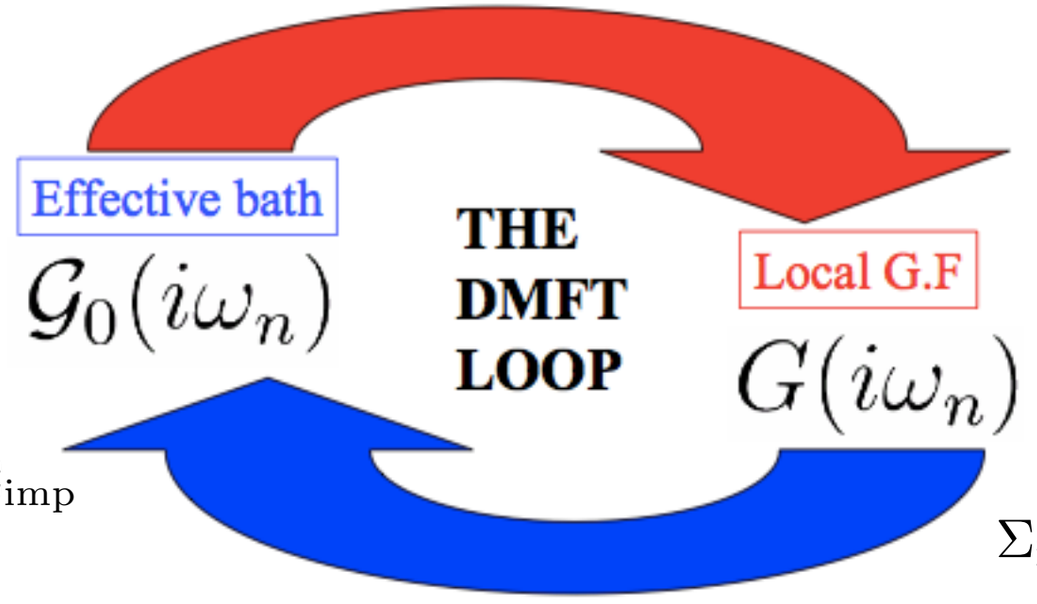
$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^{+}_\sigma(\tau) \mathcal{G}_0^{-1}(\tau - \tau') c_\sigma(\tau') + U \int_0^\beta d\tau\, n_\uparrow(\tau) n_\downarrow(\tau)$$

$$\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \varepsilon_0 - \Delta(i\omega_n)$$

$$\Sigma_{ii} \simeq \Sigma_{imp} \ , \ \Sigma_{i\neq j} \simeq 0$$

this is the computationally difficult part

EFFECTIVE LOCAL IMPURITY PROBLEM



$$\mathcal{G}^{-1}_{0,\text{new}} = G^{-1}_{\text{loc}} + \Sigma_{\text{imp}}$$

$$\Sigma_{\text{imp}} = \mathcal{G}_0^{-1}(i\omega_n) - G^{-1}_{\text{imp}}(i\omega_n)$$

SELF-CONSISTENCY CONDITION

$$\mathcal{G}_{\text{loc}} = \sum_{\mathbf{k}} [i\omega_n + \mu - \epsilon_k - \Sigma_{\text{imp}}(i\omega_n)]^{-1}$$

DMFT

DMFT becomes exact in the following limits:

- non-interacting limit $U = 0$ (no selfenergy)
- atomic limit $t=0$ (all sites effectively decoupled)
- infinite coordination number z, with properly scaled hoppings

I view DMFT as an *interpolation* technique between the U=0 and t=0 limits, satisfying the limit of infinite coordination number.

DMFT in physics

Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions

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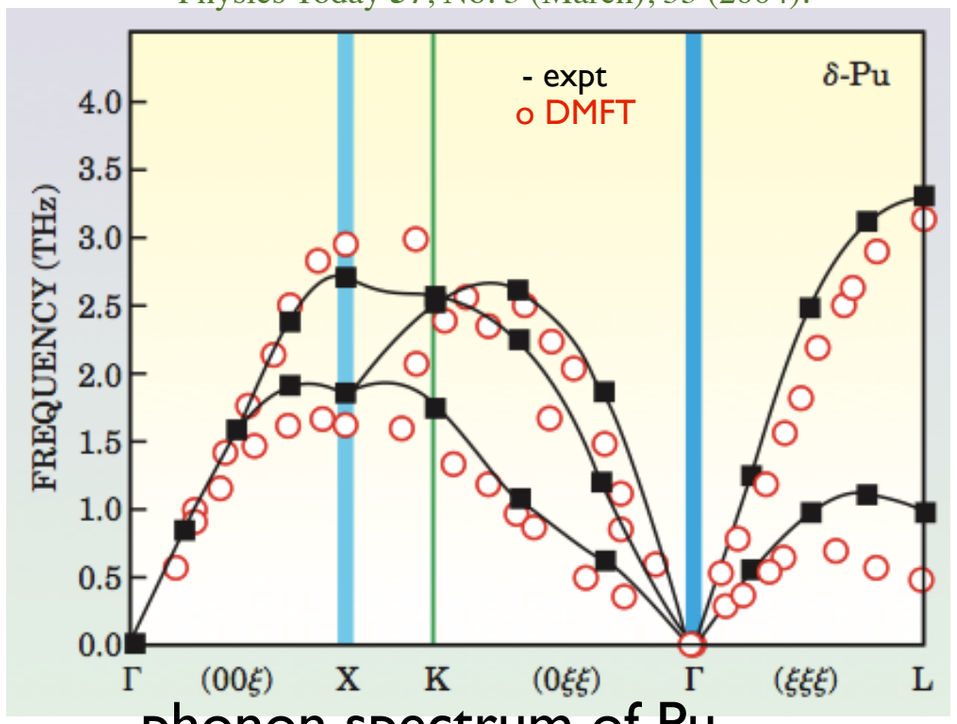
G. Kotliar and D. Vollhardt, Strongly Correlated Materials: Insights from Dynamical Mean-Field Theory Physics Today **57**, No. 3 (March), 53 (2004).



phonon spectrum of Pu

X. Dai et al., Science **300**, 953 (2003);. J. Wong et al., Science **301**, 1078 (2003).

Electronic structure calculations with dynamical mean-field theory

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Department of Physics and Astronomy and Center for Condensed Matter Theory, Rutgers University, Piscataway, New Jersey 08854-8019, USA; Service de Physique Theorique, CEA Saclay, 91191 Gif-Sur-Yvette, France; and Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau Cedex, France

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Quantum cluster theories

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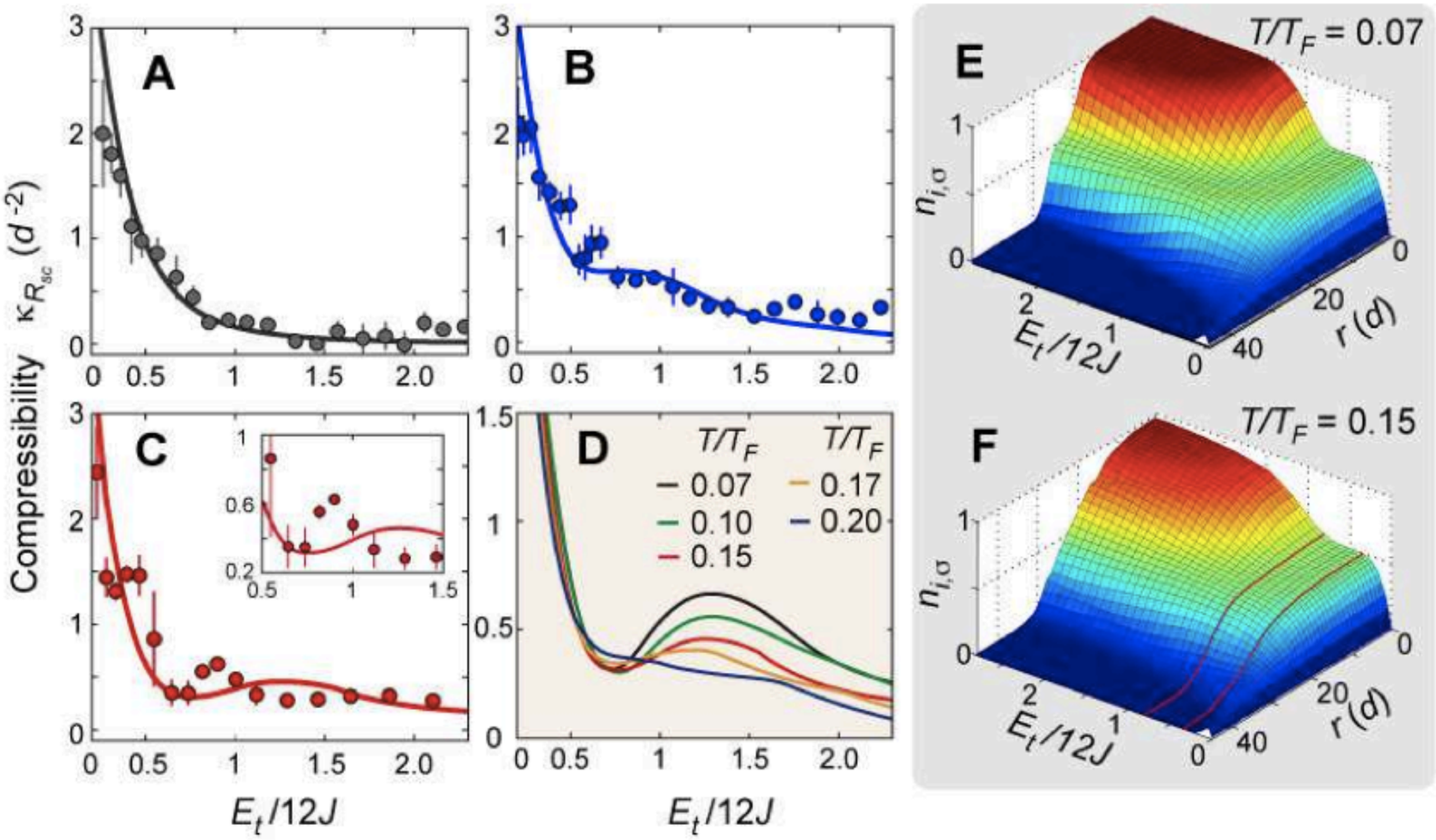
DMFT in cold gases



$$E_t = V_t(\gamma N_\sigma/(4\pi/3))^{2/3}$$

$$\gamma = \omega_z/\omega_\perp$$

$$R_{sc} = \frac{\sqrt{r_\perp^2}}{(\gamma N_\sigma)^{1/3}}$$

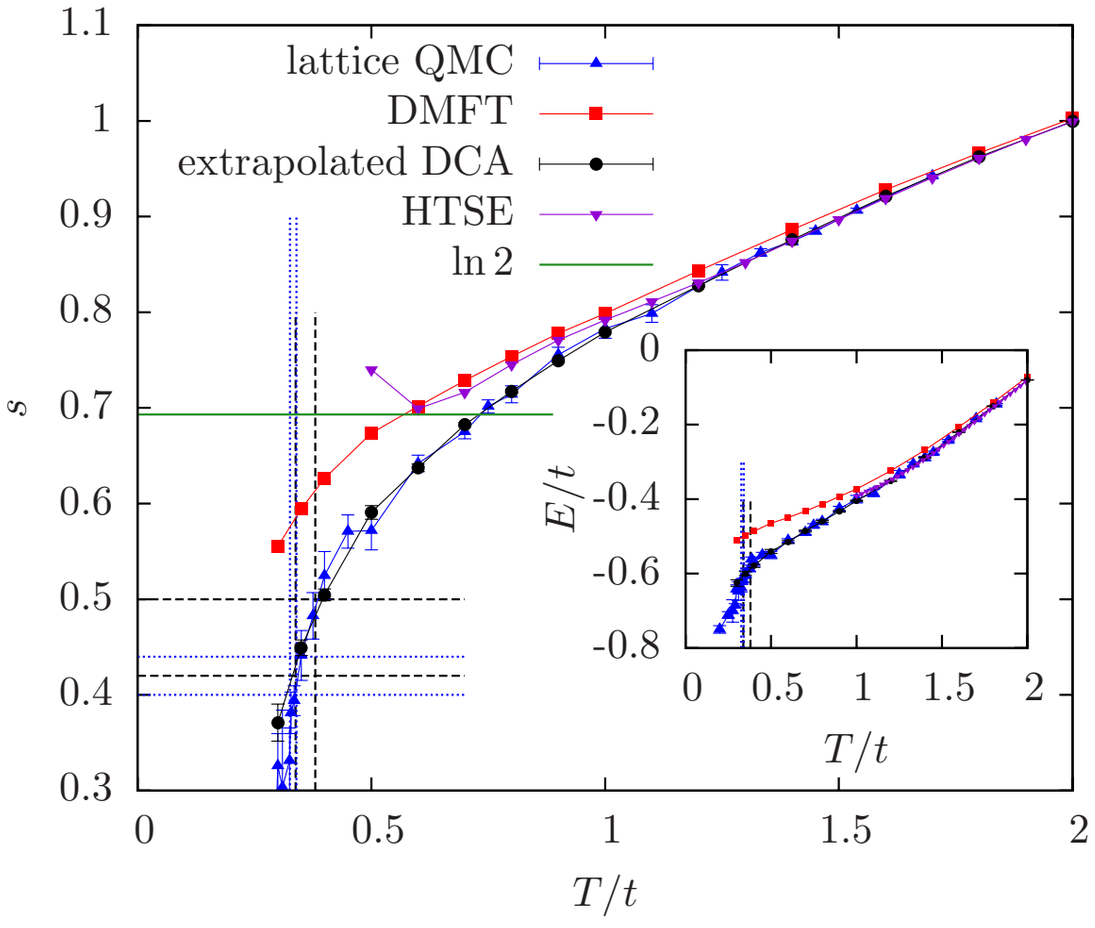
$$\kappa_{R_{sc}} = -\frac{1}{R_{sc}^3}\frac{\partial R_{sc}}{\partial(E_t/12J)}$$

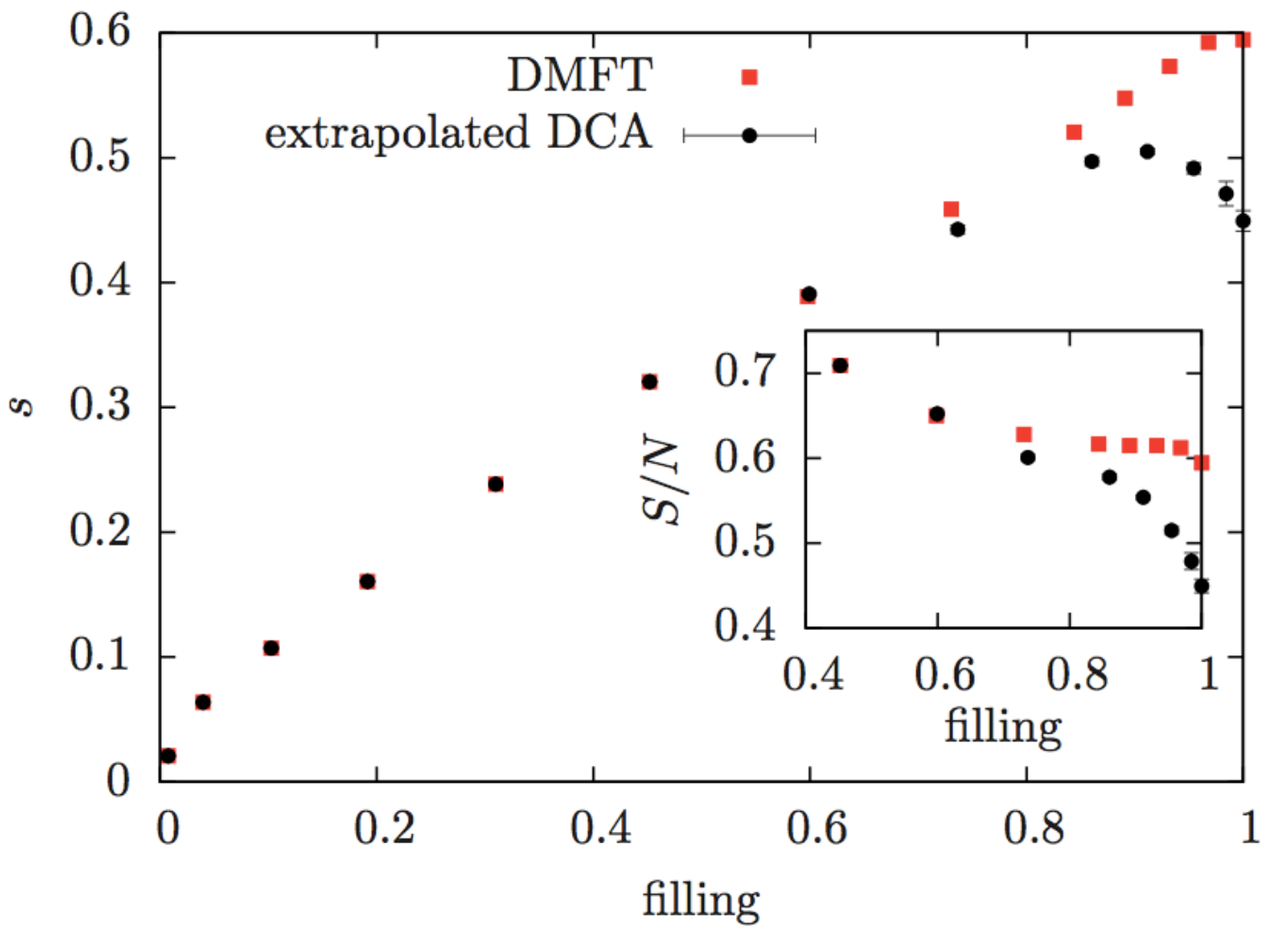
U. Schneider *et al*., Science, Vol. **322**, p.1520-1525 (2008).

groups of A. Rosch, N. Blümer , A. Georges, W. Hofstetter, ...
also applied DMFT (or small variants) to cold gases

cold gases beyond DMFT

3d Hubbard model, U=8, half filling, physics on approach to T_N





S.Fuchs, E. Gull, L. Pollet, E. Burovski, E. Kozik, T. Pruschke, and M. Troyer, arXiv:1009.2759 (2010).

when experiments reach colder temperature, we will reach a point where the physics is no longer accurately described by DMFT

see also the talk by Emanuel Gull later in this program!

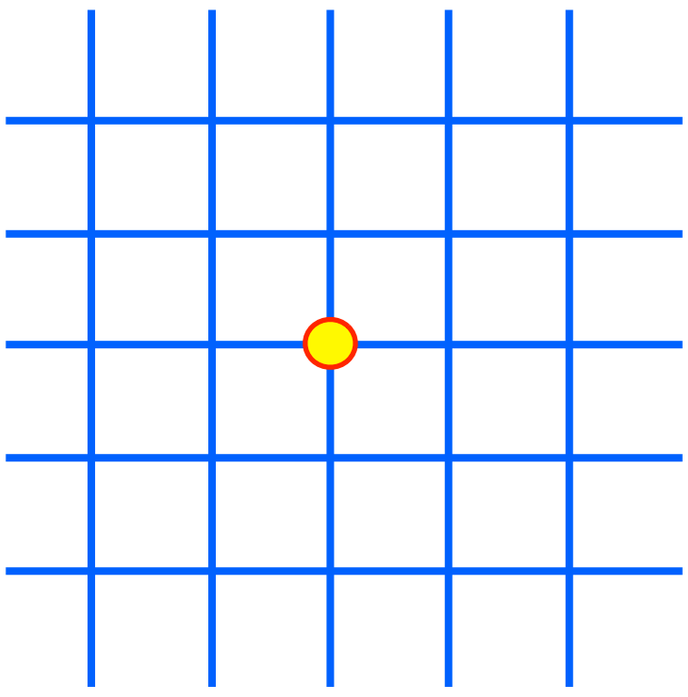
E. Gull *et al.*, arXiv:1010.3690 (2010).

Goal

We want to develop the dynamical mean-field solution for the 3d Bose-Hubbard model

$$H = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i$$

write down single-site action :



$$S_{\text{imp}} = \int_0^\beta d\tau b^\dagger(\tau) \left[\partial_\tau - \mu\right] b(\tau) + \frac{U}{2} \int_0^\beta d\tau n(\tau) \left[n(\tau) - 1\right]$$

we lost the momentum dependence for the self-energy

works fine for normal phase and Mott phase.

we want:
include the physics of the weakly interacting Bose gas non-perturbatively,
which is the limit t >>U

we want: correction on top of mean-field

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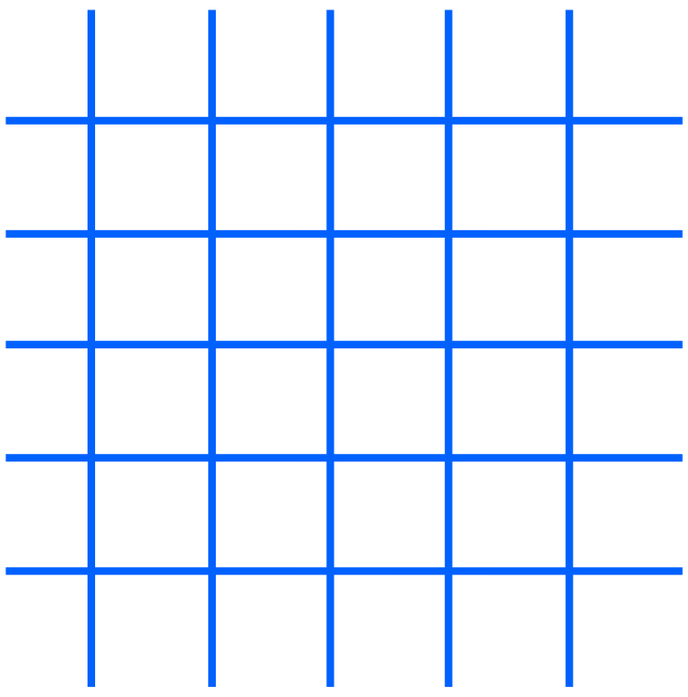

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Weakly interacting Bose gas

B. Capogrosso-Sansone, S. Giorgini, S. Pilati, L. Pollet, N. V. Prokof'ev, B. V. Svistunov, and M. Troyer, New J. Phys. **12**, 043010 (2010)

continuous space description:

$$H = H_0 + H_{\rm int} + H_1$$

$$H_0 = \frac{1}{2m}\int |\nabla\psi|^2 \mathrm{d}\mathbf{r}$$

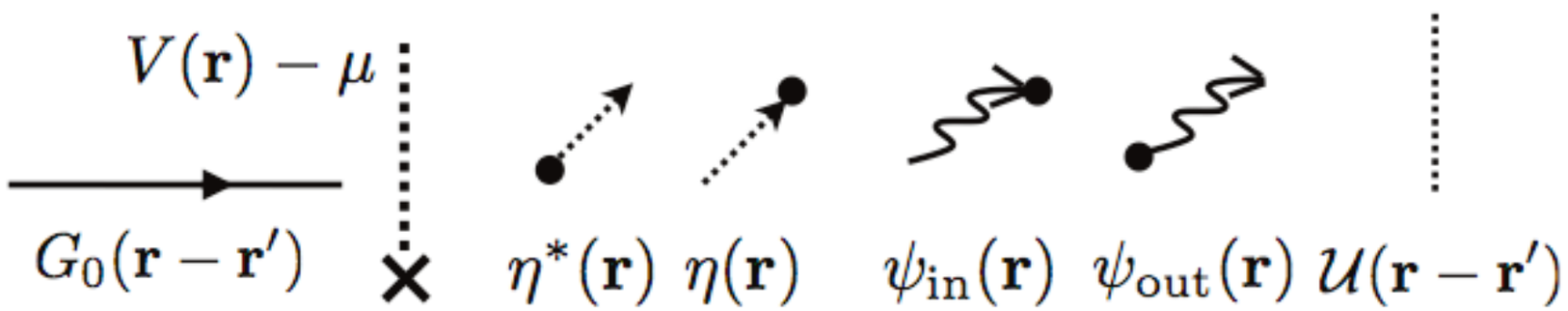
$$G^{(0)}(\xi,\mathbf{k}) = \frac{1}{i\xi - \epsilon(k)}$$

$$H_{\rm int} = \frac{1}{2}\int \mathcal{U}(\mathbf{r}_1-\mathbf{r}_2)|\psi(\mathbf{r}_1)|^2|\psi(\mathbf{r}_2)|^2 \mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2$$

$$H_1 = \int [V(\mathbf{r})-\mu]|\psi|^2\mathrm{d}\mathbf{r} - \int [\eta^*\psi + \mathrm{c.c.}]\,\mathrm{d}\mathbf{r}$$

not in non-interacting Hamiltonian; effect is non-perturbative because μ is negative for ideal gas and positive for WIBG

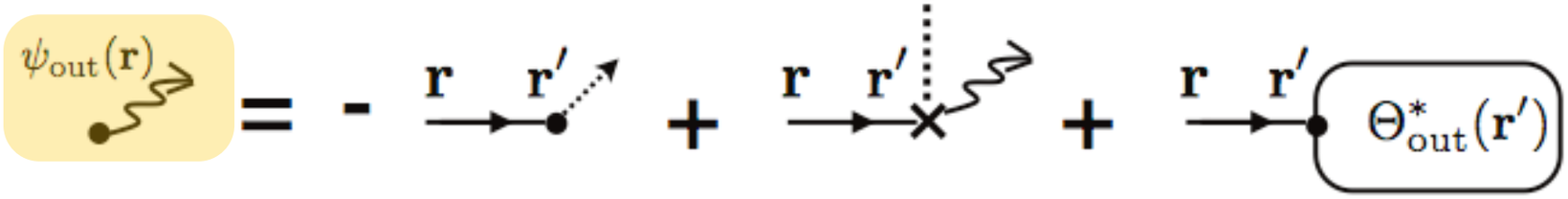
symmetry explicitly *broken*; introduces gap and stabilizes supercurrent states

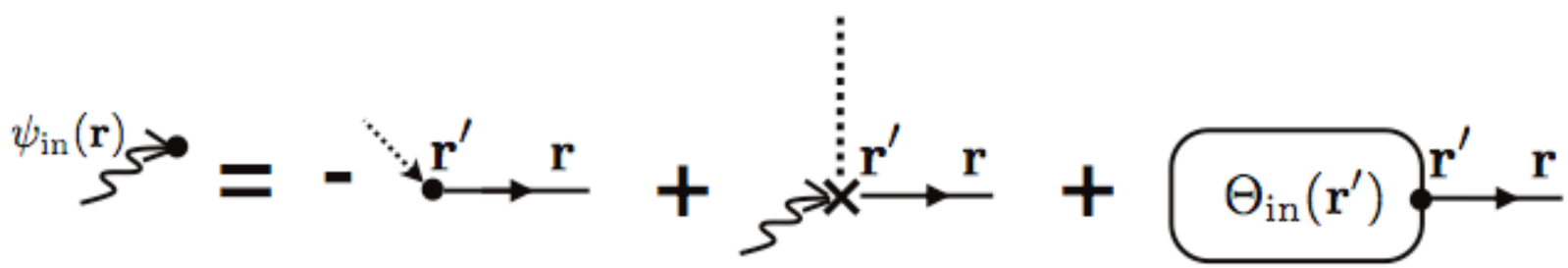


Weakly interacting Bose Gas

B. Capogrosso-Sansone, S. Giorgini, S. Pilati, L. Pollet, N. V. Prokof'ev, B. V. Svistunov, and M. Troyer, New J. Phys. **12**, 043010 (2010)

consider number-breaking diagrams with only one incoming or outgoing line (= due to η only)





$$\psi_{\rm in}(\mathbf{r}) = -G^{(0)}(\mathbf{r}-\mathbf{r}')\eta(\mathbf{r}') + G^{(0)}(\mathbf{r}-\mathbf{r}')[V(\mathbf{r}')-\mu]\psi_{\rm in}(\mathbf{r}') + G^{(0)}(\mathbf{r}-\mathbf{r}')\Theta_{\rm in}(\mathbf{r}')$$

$$\psi_{\rm out} = \psi^*_{\rm in}\,, \qquad \Theta_{\rm out} = \Theta^*_{\rm in}$$

diagrammatic expansion for anomalous average (=condensate wavefunction)

$$\psi_0(\mathbf{r}) = \langle\psi(\mathbf{r})\rangle \equiv \psi_{\rm in}(\mathbf{r})$$

condensate density

$$n_0(\mathbf{r}) = |\psi_0(\mathbf{r})|^2$$

Greens function is resolvent of Laplace operator

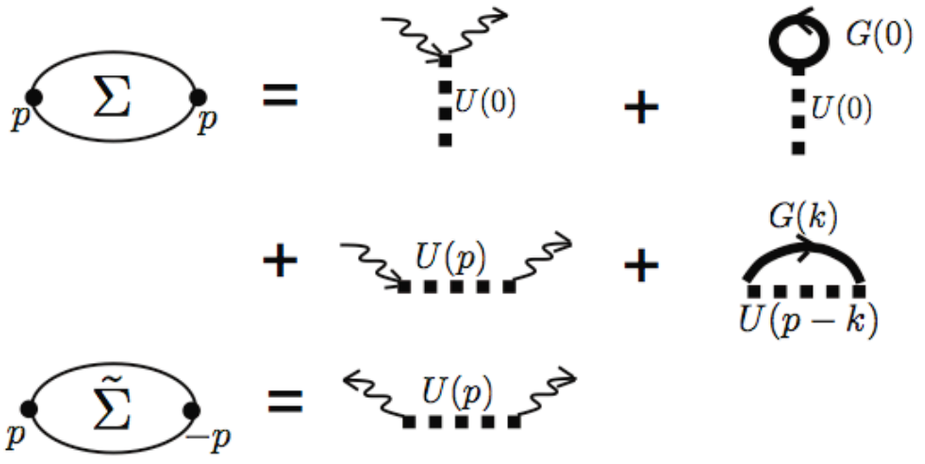
$$-\frac{\Delta}{2m}\psi_0(\mathbf{r}) + [V(\mathbf{r})-\mu]\psi_0(\mathbf{r}) + \Theta_{\rm in}(\mathbf{r}) = \eta(\mathbf{r})$$

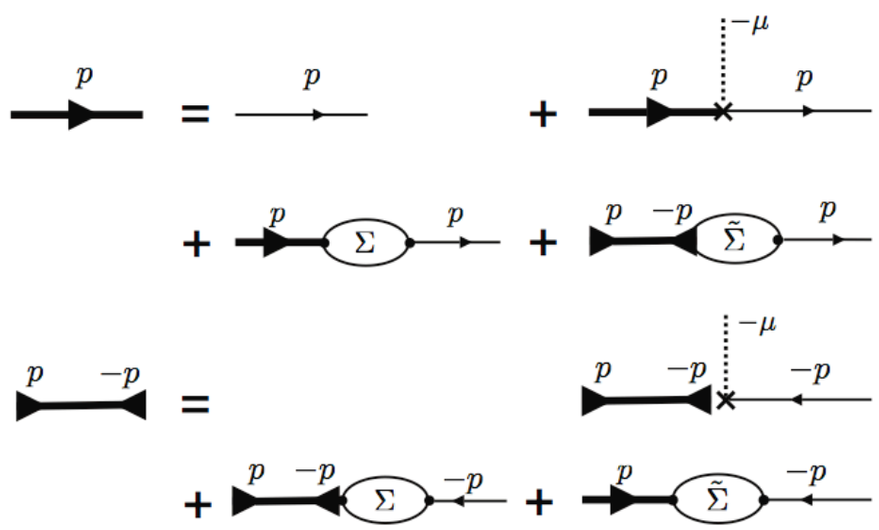
in homogeneous case

$$\mu = \Theta_{\rm in}/\psi_0 \equiv \Theta_{\rm out}/\psi^*_0$$

weakly interacting Bose gas

Why BDMFT should be good: look at self-energies of weakly interacting Bose gas (Beliaev)





$$\Sigma(P) = -2G(r=0,\tau=-0)U + 2n_0U = 2nU$$

$$\tilde{\Sigma}(P) = n_0U\ .$$

momentum independent to leading and subleading order

B. Capogrosso-Sansone, S. Giorgini, S. Pilati, L. Pollet, N. V. Prokof'ev, B. V. Svistunov, and M. Troyer, New J. Phys. **12**, 043010 (2010)

$$G(P) = -\frac{\mathrm{i}\xi + \epsilon(k) + |\tilde{\mu}|}{\xi^2 + E^2(k)}$$

$$F(P) = \frac{|\tilde{\mu}|}{\xi^2 + E^2(k)}\ ,$$

similar in magnitude at low temperature, but opposite in sign

$$E^2(k) = \epsilon(k)[\epsilon(k) + 2|\tilde{\mu}|]$$

$$\tilde{\mu} = \mu - 2nU$$

Hohenberg P C and Martin P C 1965 Ann. Phys. 34 291
Hugenholtz N M and Pines D S 1959 Phys. Rev. 116 489
Nepomnyashchii A A and Nepomnyashchii Yu A 1978 Zh. Eksp. Teor. Fiz. 75 976 [1978 Sov. Phys. JETP 48 493]
Nepomnyashchii Yu A 1983 Zh. Eksp. Teor. Fiz. 85 1244 [1983 Sov. Phys. JETP 58 722]

Hugenholtz-Pines

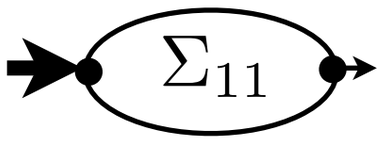
B. Capogrosso–Sansone, S. Giorgini, S. Pilati, L. Pollet, N. V. Prokof'ev, B. V. Svistunov, and M. Troyer, New J. Phys. **12**, 043010 (2010)

Recall : Θ_{in} is the sum of all diagrams attached to a bare green function other than μ or η^*

Let $D^{(l)}$ sum of diagrams contributing to Θ_{in} with l incoming and $(l\text{-}1)$ outgoing condensate lines

We had before: $$-\frac{\Delta}{2m}\psi_0(\mathbf{r}) + [V(\mathbf{r}) - \mu]\psi_0(\mathbf{r}) + \Theta_{\rm in}(\mathbf{r}) = \eta(\mathbf{r})$$

$$\mu = \Theta_{\rm in}/\psi_0 \equiv \Theta_{\rm out}/\psi_0^*$$



Dress Σ_{11} with ψ_0 : it becomes a term contributing to Θ_{in}

Say Σ_{11} has (k-1) incoming condensate lines; upon integration with ψ_0 it contributes to $D^{(k)}$

How many such diagrams are there? Answ : k

$$\Sigma_{11}(\mathbf{r},\mathbf{r}')\psi_0(\mathbf{r}') = \sum_{l=1}^{\infty} l D^{(l)}$$

similarly:

$$\Sigma_{02}(\mathbf{r},\mathbf{r}')\psi_0^*(\mathbf{r}') = \sum_{l=2}^{\infty} (l-1) D^{(l)}$$

homogeneous $\eta \to 0$

$$\mu = \Sigma_{11}(0,0) - \Sigma_{02}(0,0)$$

if $\eta = zt\psi_0$

$$\mu = \Sigma_{11}(0,0) - \Sigma_{02}(0,0) - zt$$

Recap

We want to develop the dynamical mean-field solution for the 3d Bose-Hubbard model

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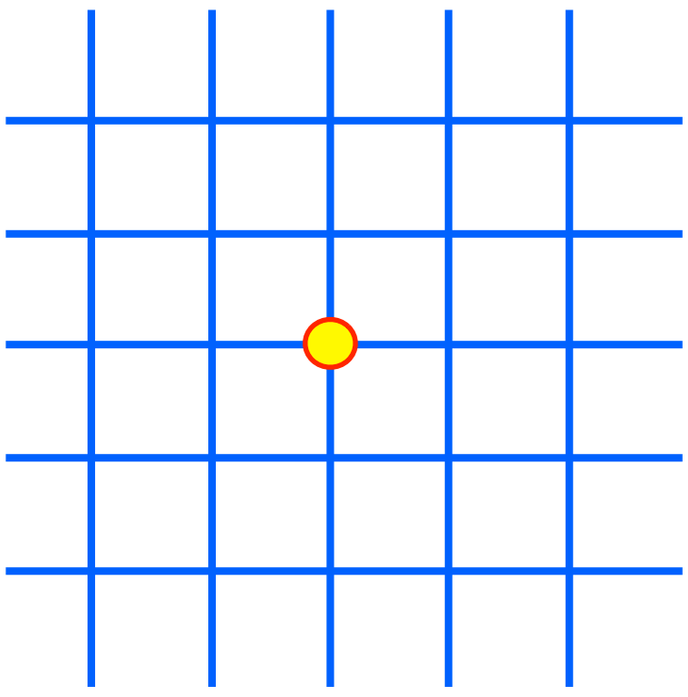
write down single-site action :



$$S_{\text{imp}} = \int_0^\beta d\tau b^\dagger(\tau) \left[\partial_\tau - \mu\right] b(\tau) + \frac{U}{2} \int_0^\beta d\tau n(\tau) \left[n(\tau) - 1\right]$$

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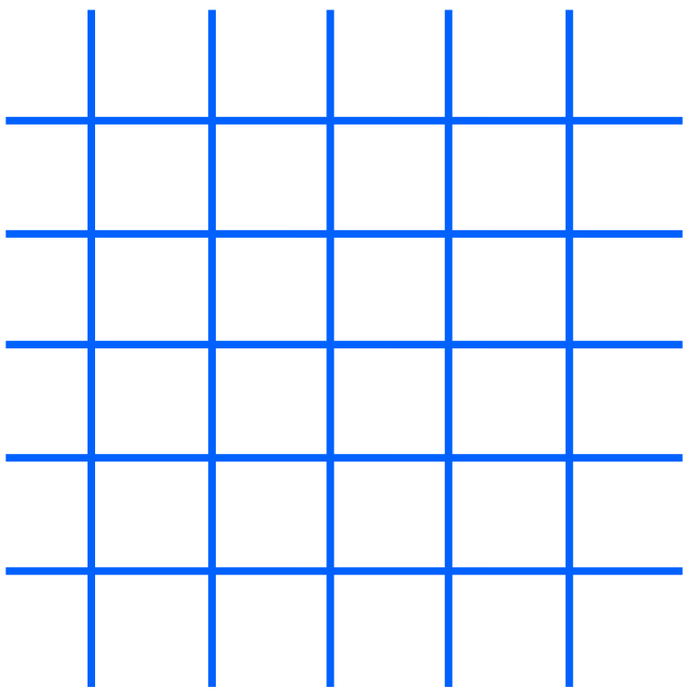

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source fields

let's add a symmetry breaking field :

$$-zt\phi \int_0^\beta d\tau [b(\tau) + b^\dagger(\tau)]$$

this is the same as in static mean-field which can produce a condensate

Bogoliubov prescription : $b(\tau) = \langle b \rangle + \delta b(\tau)$

imag time dynamics can be added in the two-particle channel.
The second source field can only couple to the normal bosons, otherwise *double counting* will occur (Nambu notation):

for infinite coordination number, this term is *zero*

$$-\frac{1}{2} \int_0^\beta d\tau d\tau' \delta \mathbf{b}^\dagger(\tau) \mathbf{\Delta}(\tau - \tau') \delta \mathbf{b}(\tau')$$

which contains normal and anomalous propagators.

see J.W. Negele and H. Orland, Quantum Many-Particle Systems (Addison-Wesley Publishing Company 1988) ISBN 0-201-12593-5 for how to treat broken symmetry

Final step : re-express δb in terms of full b

mean-field theory for bosons

$$Z = Z_0 \int \prod_i D\psi_i(\tau) D\psi_i^*(\tau) \exp[-S(\psi_i)] , \qquad \text{(A3)}$$

with an effective action

$$S(\psi_i) = \sum_{i,j} \int d\tau (J^{-1})_{ij} \psi_i^*(\tau) \psi_j(\tau) - \sum_i \ln \left\langle T_\tau \exp \left[\int d\tau \, \psi_i(\tau) \hat{\Phi}_i^+(\tau) + \text{H.c.} \right] \right\rangle_0 , \qquad \text{(A4)}$$

where $(J^{-1})_{ij}$ is the inverse of the matrix of hopping rates. The average in (A4), which is now on-site in the original boson field Φ_i, can be readily computed as a cumulant expansion in powers of ψ_i. Since $\langle \psi_i \rangle$ is linearly related to $\langle \Phi_i \rangle$, the field ψ_i serves as an order parameter for superfluidity.

= after Hubbard-Stratonovich transform in the hopping (strong-coupling expansion)

Equations (A3) and (A4) represent an exact rewriting of the original partition function and thereby serves as a convenient starting point to generate a field theoretic description of the onset of superfluidity (see Sec. IV A). Here, we pursue a different path, specializing to the infinite-range hopping limit of (2.1), namely $J_{ij} \equiv J/N$, where N is the total number of lattice sites in the system. In this limit H_1 can be expressed as a perfect square,

$$H_1 = -(J/N) \left[\sum_i \hat{\Phi}_i^+ \right] \left[\sum_i \hat{\Phi}_i \right] \qquad \text{(A5)}$$

and only a single auxiliary field $\psi(\tau)$ is needed to decouple the nonlocal hopping term. The action in (A4) then takes the form $S_\infty(\psi) = N f(\psi)$, so that in the thermodynamic limit a saddle point evaluation of the functional integral in (A3) becomes exact. With the assumption that the lowest-energy saddle point solution involves a time independent field, $\psi(\tau) = \psi$, one finds upon performing the cumulant expansion in (A4) an action of the typical Landau form

$$S_\infty(\psi) = \beta N [\tfrac{1}{2} r(\mu, J, T) |\psi|^2 + u(\mu, T) |\psi|^4 + O(|\psi|^6)] .$$

excerpt from Appendix A in Matthew P. A. Fisher, Peter B. Weichman, G. Grinstein, and Daniel S. Fisher, Phys. Rev. B **40**, 546 (1989)

...

the BDMFT approximation

Missing are still the selfconsistency equations.

There are (more than) 3 ways to proceed:

- effective medium/RG-like description — will be done in this talk
- cavity method — will be outlined in this talk
- kinetic energy functional approximation and coupling constant integration method

= the most elegant method,
see EPAPS material in PRL paper for full treatment

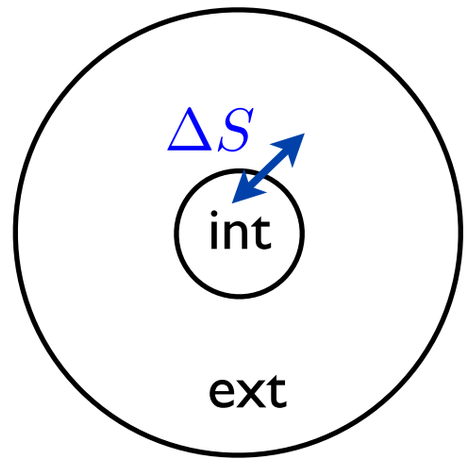
real-space RG reasoning to find the action

$$Z = \int \mathcal{D}[b_j^*, b_j] \exp(-S[b_j^*, b_j]) \qquad S = S_{\rm int} + \Delta S + S_{\rm ext}$$

$$S_{\rm int} = \int_0^\beta d\tau b_{\rm int}^*(\tau)(\partial_\tau - \mu) b_{\rm int}(\tau) + \frac{U}{2} n_{\rm int}(n_{\rm int} - 1).$$

$$\Delta S = \int_0^\beta \Delta S(\tau) = \int_0^\beta \sum_{\langle {\rm int}, {\rm ext}\rangle} -t \left(b_{\rm int}^\dagger b_{\rm ext} + b_{\rm ext}^\dagger b_{\rm int} \right)$$

$$S_{\rm ext} = \int_0^\beta d\tau b_{\rm ext}^*(\tau)(\partial_\tau - \mu) b_{\rm ext} + \frac{U}{2} n_{\rm ext}(n_{\rm ext} - 1).$$



$$b_{\rm ext} = \phi_{\rm ext} + \delta b_{\rm ext}$$ spontaneously broken

$$b_{\rm int} = \phi_{\rm int} + \delta b_{\rm int}, \quad \langle b_{\rm int} \rangle = \phi_{\rm int}$$ through hopping events in 'ext'

goal : derive an effective action for the impurity 'imp' with parameters self-consistently determined by the 'bath' (so integrate out ΔS)

cf. Section IIID in A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13-125 (1996).

real-space RG

We can exactly rewrite:

$$\Delta S = \int_0^\beta \sum_{\langle \mathrm{int,ext}\rangle} -t\left(b^\dagger_{\mathrm{int}} b_{\mathrm{ext}} + b^\dagger_{\mathrm{ext}} b_{\mathrm{int}}\right)$$

$$= -t\int_0^\beta d\tau z\phi_{\mathrm{int}}(\delta b_{\mathrm{ext}} + \delta b^\dagger_{\mathrm{ext}}) + z\phi_{\mathrm{ext}}(\delta b_{\mathrm{int}} + \delta b^\dagger_{\mathrm{int}})$$

$$+ \sum_{\langle \mathrm{int,ext}\rangle} \delta b^\dagger_{\mathrm{int}}\delta b_{\mathrm{ext}} + \delta b^\dagger_{\mathrm{ext}}\delta b_{\mathrm{int}},$$

We keep in the exponent:

$$S_1 = zt\phi_{\mathrm{ext}} \int \delta b(\tau) + \delta b^\dagger(\tau) = zt\phi_{\mathrm{ext}} \int b(\tau) + b^\dagger(\tau)$$

and expand only in the term (the other one factorizes):

$$\Delta S = -t\int_0^\beta \sum_{\langle \mathrm{int,ext}\rangle} \delta b^\dagger_{\mathrm{int}}\delta b_{\mathrm{ext}} + \delta b^\dagger_{\mathrm{ext}}\delta b_{\mathrm{int}}$$

N.B. if you do not introduce the condensate on the 'int' part at this point but expand into the full b-operators (instead of δb) , you will have to reintroduce the condensate and bring it back into the exponent (=identify all the diagrams to all orders contributing to the condensate). This is doable (cf. the weakly interacting Bose gas), but a bit more technical than the approach followed here and making life unnecessarily complicated

real-space RG

this results in an infinite series:

$$Z \sim Z^{\rm ext} \int D[b^*_{\rm int}, b_{\rm int}] e^{-S_{\rm int}[b^*_{\rm int}, b_{\rm int}] - S_1[b^*_{\rm int}, b_{\rm int}]\zeta}$$

$$\zeta = 1 - \int_0^\beta d\tau \langle \Delta S(\tau) \rangle_{\rm ext} +$$

$$+ \frac{1}{2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle \Delta S(\tau_1) \Delta S(\tau_2) \rangle_{\rm ext} + \ldots$$

We will now examine what these terms look like.

to first order :

$$\int_0^\beta \langle \Delta S \rangle_{\rm ext} = -t \int_0^\beta d\tau \sum_{\langle {\rm int, ext} \rangle} \langle \delta b^\dagger_{\rm int} \delta b_{\rm ext} \rangle_{\rm ext} + {\rm h.c.}$$

is zero

real-space RG

to second order :

$$\frac{1}{2}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle \Delta S(\tau_1)\Delta S(\tau_2)\rangle_{\rm ext} =$$
$$\frac{t^2}{2}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{j,k\in{\rm ext}} [S^1 + S^2 + S^3 + S^4].$$

with:

$$S^1 = \langle \delta b_{\rm int}(\tau_1)\delta b_{\rm int}(\tau_2)\delta b^{\dagger(j)}_{\rm ext}(\tau_1)\delta b^{\dagger(k)}_{\rm ext}(\tau_2)\rangle_{\rm ext}$$
$$S^2 = \langle \delta b_{\rm int}(\tau_1)\delta b^\dagger_{\rm int}(\tau_2)\delta b^{\dagger(j)}_{\rm ext}(\tau_1)\delta b^{(k)}_{\rm ext}(\tau_2)\rangle_{\rm ext}$$
$$S^3 = \langle \delta b^\dagger_{\rm int}(\tau_1)\delta b_{\rm int}(\tau_2)\delta b^{(j)}_{\rm ext}(\tau_1)\delta b^{\dagger(k)}_{\rm ext}(\tau_2)\rangle_{\rm ext}$$
$$S^4 = \langle \delta b^\dagger_{\rm int}(\tau_1)\delta b^\dagger_{\rm int}(\tau_2)\delta b^{(j)}_{\rm ext}(\tau_1)\delta b^{(k)}_{\rm ext}(\tau_2)\rangle_{\rm ext}.$$

in the presence of a condensate, the anomalous terms
are also nonzero.

real-space RG

cumulant re-exponentiation

$$e^{-S_2^1} = e^{-\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \delta b_{\rm int}(\tau_1) K_c(\tau_1-\tau_2) \delta b_{\rm int}(\tau_2)}$$ and analogous for the 3 other terms

we could go on, but we are already in a position to postulate the form of the effective impurity action:

$$S_{\rm imp} = \int_0^\beta d\tau b^*_{\rm int}(\tau)(\partial_\tau - \mu) b_{\rm int}(\tau) + \frac{U}{2} n_{\rm int}(n_{\rm int}-1)$$

$$-zt\mathbf{\Phi}^\dagger_{\rm ext} \int_0^\beta d\tau \mathbf{b}_{\rm int}(\tau)$$

$$+ \int_0^\beta d\tau \int_0^\beta d\tau' (\mathbf{b}^\dagger_{\rm int}(\tau) - \mathbf{\Phi}_{\rm int}(\tau)) \mathbf{\Delta}(\tau-\tau') (\mathbf{b}_{\rm int}(\tau') - \mathbf{\Phi}_{\rm int}(\tau'))$$

notation: $$\mathbf{\Delta}(\tau-\tau') = \begin{pmatrix} F(\tau'-\tau) & 2K(\tau-\tau') \\ 2K^*(\tau-\tau') & F(\tau-\tau') \end{pmatrix}$$

F, K and ϕ have to be determined self-consistently:

the condensate has to be the same on all sites: $$\phi = \phi_{\rm ext} = \phi_{\rm int} = \langle b \rangle_{\rm int}$$

normal and anomalous Green function treated similarly as in fermionic DMFT: (= the Green's function on the impurity coincides with the local Green function of the medium)

$$\mathbf{G}_{\rm latt}(i\omega_n) = \sum \left[i\omega_n \sigma_3 + (\mu - \epsilon_{\mathbf{k}})\mathbf{1} - \mathbf{\Sigma}(i\omega_n) \right]^{-1}$$

$$\mathbf{G}_{\rm latt}(i\omega_n) = \int d\epsilon D(\epsilon) (i\omega_n \sigma_3 + (\mu-\epsilon)\mathbf{I} - \mathbf{\Sigma}(i\omega_n))^{-1}$$

real-space RG

the effective action can be rewritten as:

$$S_{\rm imp} = -\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' \mathbf{b}^\dagger(\tau)\mathbf{G}_0^{-1}(\tau-\tau')\mathbf{b}(\tau') + \frac{U}{2}\int_0^\beta d\tau n(\tau)[n(\tau)-1] - \kappa\mathbf{\Phi}^\dagger\int_0^\beta d\tau \mathbf{b}(\tau).$$

Nambu notation

with:

$$\mathbf{\Delta}(i\omega_n) = -i\omega_n\sigma_3 - \tilde{\mu}\mathbf{1} + \mathbf{G}_0^{-1}(i\omega_n)$$

$$\kappa = zt - F(i\omega_n = 0) - K(i\omega_n = 0) - K^*(i\omega_n = 0)$$

or, written out in components:

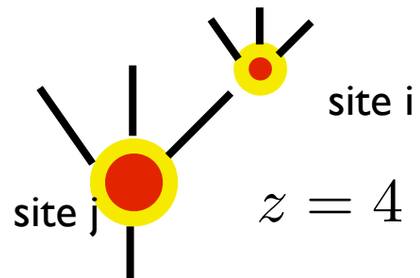
$$S_{\rm imp} = -\int_0^\beta d\tau d\tau' \left[b(\tau)F(\tau-\tau')b^\dagger(\tau') + b^\dagger(\tau)K(\tau-\tau')b^\dagger(\tau') + b(\tau)K^*(\tau-\tau')b(\tau')\right] + \int_0^\beta b^\dagger(tau)(\partial_\tau - \mu)b(\tau) + \frac{U}{2}\int_0^\beta d\tau n(\tau)[n(\tau)-1] - \kappa\int_0^\beta d\tau[\phi^* b(\tau) + \phi b^\dagger(\tau)]$$

1/z expansion

On a Bethe lattice (= Cayley tree) Semerjian *et al.* show that :

- with a coherent path integral representation, the exact solution reduces to mean-field theory for infinite coordination number and to BDMFT in first order 1/z
- with a number occupation representation, the exact solution can be written as a selfconsistency equation

idea ('cavity method'):
use recursive structure of the tree



$Z_{i\text{-}j}$ is partial partition function of subtree rooted at site i, excluding the branch between i and j for fixed occupation number on site i. This can be normalized and leads to probabilities η.

Requiring that all edges and all vertices are equal leads to the self-consistency equation:

$$\eta_{\rm cav}(b^*,b) = \frac{1}{Z_{\rm cav}} w(b^*,b) \int \prod_{i=1}^{z-1} \mathcal{D}[b_i^*,b_i] \eta_{\rm cav}(b_i^*,b_i) \exp\left[t \int_0^\beta d\tau \left(b^*(\tau) \sum_i^{z-1} b_i(\tau) + b(\tau) \sum_{i=1}^{z-1} b_i^*(\tau) \right) \right]$$

with weights:

$$w(b^*,b) = \exp\left[-\int_0^\beta d\tau \left(b^*(\tau)(\partial_\tau - \mu) b(\tau) + \frac{U}{2} n(\tau)(n(\tau)-1) \right) \right]$$

G. Semerjian, M. Tarzia, and F. Zamponi, Phys. Rev. B **80**, 014524 (2008).

1/z expansions

This can be rewritten using the generating functional Γ and in Nambu notation:

$$\eta_{\rm cav}(\mathbf{b}) = \frac{1}{Z_{\rm cav}} w(\mathbf{b}) e^{(z-1)\Gamma(t\mathbf{b})},$$

$$\Gamma(\mathbf{\Phi}) = \ln\left[\int \mathcal{D}\mathbf{b}\eta_{\rm cav}(\mathbf{b}) \exp\int_0^\beta d\tau \mathbf{b}^\dagger(\tau)\mathbf{\Phi}(\tau)\right]$$

The generating functional of connected correlation functions can safely be expanded as:

$$\Gamma(\mathbf{\Phi}) = \int_0^\beta d\tau \langle \mathbf{b}^\dagger\rangle_{\rm cav}\mathbf{\Phi}(\tau) + \frac{1}{2}\int_0^\beta d\tau d\tau' \mathbf{\Phi}^\dagger(\tau)\mathbf{G}^c_{\rm cav}(\tau-\tau')\mathbf{\Phi}(\tau') + \dots$$

connected two-point correlator: $\mathbf{G}^c_{\rm cav}(\tau-\tau') = \langle \mathbf{b}^\dagger(\tau)\mathbf{b}(\tau')\rangle_{\rm cav} - \langle \mathbf{b}^\dagger(\tau)\rangle_{\rm cav}\langle \mathbf{b}(\tau')\rangle_{\rm cav}.$

Plugging the expansion for Γ into the cavity field, we get: $\eta_{\rm cav}(\mathbf{b}) = \frac{1}{Z_{\rm cav}} \exp\left[-S_{\rm cav}\right]$

with:

$$S_{\rm cav} = \frac{1}{2}\int_0^\beta d\tau d\tau' \mathbf{b}^\dagger(\tau)\mathbf{G}^{-1}_{0,\rm cav}(\tau-\tau')\mathbf{b}(\tau') + \int_0^\beta d\tau \left[\frac{U}{2}n(\tau)(n(\tau)-1) - t(z-1)\mathbf{\Phi}^\dagger_{\rm cav}\mathbf{b}(\tau)\right]$$

$$\mathbf{G}^{-1}_{0,\rm cav}(\tau-\tau') = (\partial_\tau - \mu)\sigma_3\delta(\tau-\tau') - t^2(z-1)\mathbf{G}^c_{\rm cav}(\tau-\tau')$$

G. Semerjian, M. Tarzia, and F. Zamponi, Phys. Rev. B 80, 014524 (2008).

1/z expansion

if we want to compare this with our BDMFT formalism, we need to correct for the missing leg.

for infinite coordination number z, the hopping needs to be scaled as $t \sim 1/z$. We now expand in $1/z$ to leading order.

The Green function was already accurate to this order $(t^2(z-1) \sim 1/z)$:

$$\begin{aligned}\mathbf{G}^c_{\mathrm{imp}}(\tau-\tau') &= \mathbf{G}^c_{\mathrm{cav}}(\tau-\tau') \\ &= \langle \mathbf{b}^\dagger(\tau)\mathbf{b}(\tau')\rangle_{\mathrm{imp}} - \langle \mathbf{b}^\dagger(\tau)\rangle_{\mathrm{imp}}\langle \mathbf{b}(\tau')\rangle_{\mathrm{imp}}\end{aligned}$$

The prefactor of the cavity condensate was however of order unity, *so for the impurity condensate we need to take corrections into account*

$$S_{\mathrm{imp}} = S_{\mathrm{cav}} - t\int_0^\beta d\tau \mathbf{\Phi}^\dagger \mathbf{b}(\tau).$$

$$\mathbf{\Phi}_{\mathrm{imp}} = \langle \mathbf{b}\rangle_{\mathrm{imp}} \sim \mathbf{\Phi}_{\mathrm{cav}} + t\int_0^\beta d\tau \mathbf{G}^c_{\mathrm{imp}}(-\tau)\mathbf{\Phi}_{\mathrm{cav}}.$$

inversion:

$$\boxed{\mathbf{\Phi}_{\mathrm{cav}} \sim \left(\mathbf{I} - t\mathbf{G}^c_{\mathrm{imp}}(i\omega_n = 0)\right)\mathbf{\Phi}_{\mathrm{imp}}.}$$

this part is still missing in G. Semerjian, M. Tarzia, and F. Zamponi, Phys. Rev. B **80**, 014524 (2008) but I acknowledge private discussions with these authors as well as their notes sent to me.

kinetic energy functional approximation

A. Georges, Lectures on the Physics of Highly Correlated Electron Systems VIII (2004) 3, American Institute of Physics Conference Proceedings Vol. 715, arXiv:0403123 (2004).

We perform an expansion around the *atomic limit*, use the *coupling constant integration* method, arrive at the DMFT selfconsistency equations and see what terms are neglected.

$$H_\alpha = \frac{U}{2}\sum_i n_i(n_i-1) - \alpha t \sum_{\langle i,j\rangle} b_i^\dagger b_j$$

$$\Gamma = \Gamma_{\alpha=1} = \Gamma_0 + \int_0^1 d\alpha \frac{d\Gamma_\alpha}{d\alpha}$$

Lagrange multipliers (sources) are only introduced for local quantities

functionals are obtained in the usual way by constraining the condensate and the Green function using Lagrange multipliers, demanding stationarity, and then inverting the problem expressing the source terms in terms of the constrained fields

impurity model:

local terms / source / source / source / source / source

$$\Gamma_0[\mathbf{\Phi},\mathbf{G_c}] = F_{\rm imp}[\mathbf{\Phi},\mathbf{G_c}] - \int_0^\beta d\tau [F_0(\tau)G_c(\tau) + K_0(\tau)\tilde{G}_c^*(\tau) + K_0^*(\tau)\tilde{G}_c(\tau)] + \frac{1}{N_s\beta}\int_0^\beta d\tau \sum_i [J_0^*(\tau)\phi_i(\tau) + J_0(\tau)\phi_i^*(\tau)]$$

imposed stationarity: $\mathbf{\Phi} = \langle \mathbf{b}\rangle_{S_{imp}}$

note our minus-sign convention...

$$\mathbf{G}_c(\tau) = \mathbf{G}(\tau) + \mathbf{\Phi}\mathbf{\Phi}^\dagger \qquad \mathbf{G}(\tau) = -\langle T\mathbf{b}(\tau)\mathbf{b}^\dagger(0)\rangle_{S_{\rm imp}}$$

hopping terms:

$$\frac{d\Gamma_\alpha}{d\alpha} = -\frac{1}{N_s\beta}\int_0^\beta d\tau t \sum_{\langle i,j\rangle}\langle b_i^*(\tau)b_j(\tau)\rangle = -\frac{1}{N_s\beta}\int_0^\beta d\tau t \sum_{\langle i,j\rangle}[\phi_i^*(\tau)\phi_j(\tau) + \langle \delta b_i^*(\tau)\delta b_j(\tau)\rangle]$$

$$= \frac{1}{N_s\beta}{\rm Tr}\sum_{n,\mathbf{k}}\epsilon_{\mathbf{k}}\mathbf{G}_c^\alpha(\mathbf{k},i\omega_n)|_{\mathbf{\Phi},\mathbf{G}_c} - \frac{1}{N_s\beta}\int_0^\beta d\tau t\sum_{\langle i,j\rangle}[\phi_i^*(\tau)\phi_j(\tau)].$$

kinetic energy functional approximation

A. Georges, Lectures on the Physics of Highly Correlated Electron Systems VIII (2004) 3, American Institute of Physics Conference Proceedings Vol. 715, arXiv:0403123 (2004).

The exact Green function is as always

$$\mathbf{G}_c^\alpha(\mathbf{k}, i\omega_n) = [i\omega_n\sigma_3 + (\mu - \alpha\epsilon_\mathbf{k})\mathbf{I} + \mathbf{\Delta}_\alpha[i\omega_n] - \mathbf{\Sigma}_\alpha[\mathbf{k}, i\omega_n]]^{-1}$$

in the BDMFT approximation, all Σ_α are approximated by Σ_0

$$\mathbf{G}_c^\alpha(\mathbf{k}, i\omega_n)|_{\text{B-DMFT}} = [i\omega_n\sigma_3 + (\mu - \alpha\epsilon_\mathbf{k})\mathbf{I} + \mathbf{\Delta}_\alpha[i\omega_n; \mathbf{\Phi}, \mathbf{G}_c] - \mathbf{\Sigma}_{\alpha=0}[i\omega_n; \mathbf{\Phi}, \mathbf{G}_c]]^{-1}$$

The lattice function is found by summing over all ***k***, which can be related to the hybridization function. On the basis of stationarity, one expects that $\Delta_{\alpha=1}[\boldsymbol{G}_c]=\delta\Gamma/\delta\boldsymbol{G}c=0$. The calculation confirms that this is indeed the case. Hence, we obtain the usual self-consistency equation,

$$\mathbf{G}_c(i\omega_n) = \int d\epsilon D(\epsilon)(i\omega_n\sigma_3 + (\mu - \epsilon)\mathbf{I} - \mathbf{\Sigma}_{\text{imp}}(i\omega_n))^{-1}$$

(see the EPAPS part of our paper for an explicit expression of the kinetic energy functional)
features of this approach:

- independent of U
- valid on any lattice in any dimension

N. B. This approach is DIFFERENT from the Baym-Kadanoff approach, which not only constrains *local* quantities

DMFT self-consistency loop

$$\mathbf{\Delta}(i\omega_n) = -i\omega_n\sigma_3 - \mu\mathbf{1} + \mathbf{G_0}^{-1}(i\omega_n)$$

new Quantum Monte Carlo solver (next)

1. For given $G_0(i\omega_n)$, solve the impurity problem and find $G_{\rm imp}(i\omega_n)$

2. Extract self-energy: $\Sigma_{\rm imp}(i\omega_n) = G_0^{-1}(i\omega_n) - G_{\rm imp}^{-1}(i\omega_n)$

3. DMFT approximation : $\Sigma(k, i\omega_n) = \Sigma_{\rm imp}(i\omega_n)$

$$\mathbf{G}_{\rm loc}(i\omega_n) = \sum_{\mathbf{k}} \left[i\omega_n\sigma_3 + (\mu - \epsilon_k)\mathbf{1} - \mathbf{\Sigma}_{\rm imp}(i\omega_n)\right]^{-1}$$

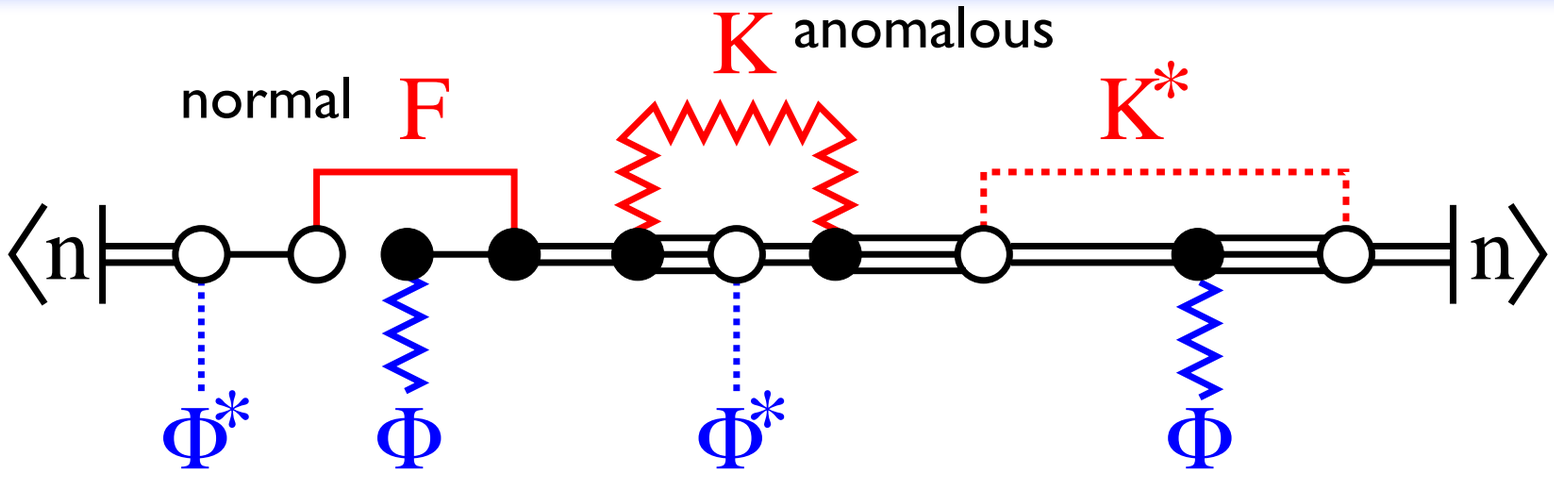
4. Define new bath $G_{0,\rm new}^{-1}(i\omega_n) = G_{\rm loc}^{-1}(i\omega_n) + \Sigma_{\rm imp}(i\omega_n)$

5.extra self-consistency condition for bosons:

$$\phi = \langle b \rangle$$

and repeat till convergence is reached

QMC impurity solver



updates:

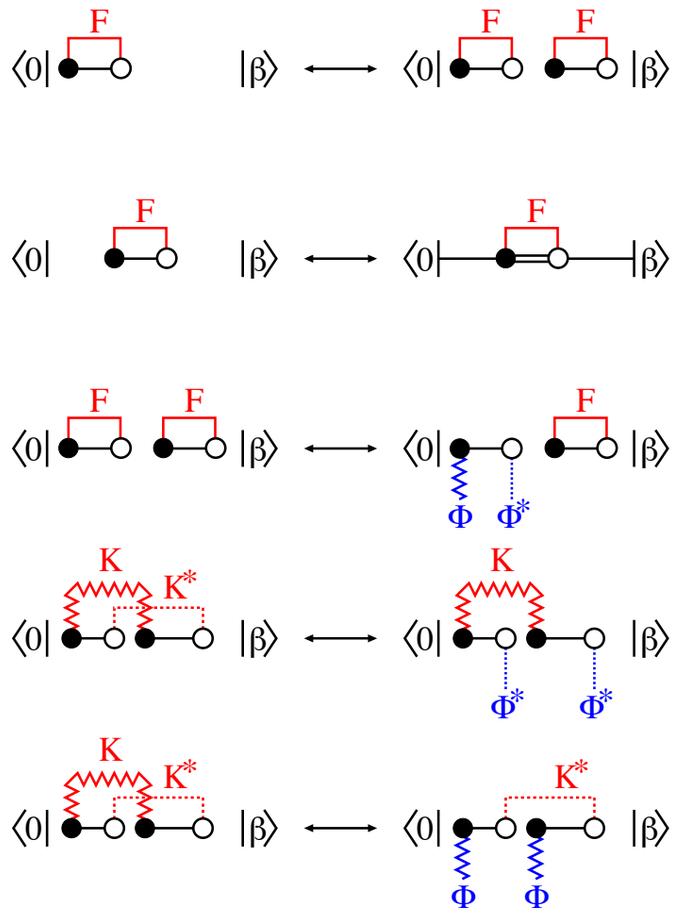
- insert F line
- change occupation nr n
- change of type:

$$b(\tau)F(\tau-\tau')b^\dagger(\tau') \leftrightarrow \kappa\phi^* b(\tau)\kappa\phi b^\dagger(\tau'),$$
$$b(\tau)K^*(\tau-\tau')b(\tau') \leftrightarrow \kappa\phi^* b(\tau)\kappa\phi^* b(\tau'),$$
$$b^\dagger(\tau)K(\tau-\tau')b^\dagger(\tau') \leftrightarrow \kappa\phi b^\dagger(\tau)\kappa\phi b^\dagger(\tau').$$

measurement:

$$\langle b(\tau)b^\dagger(0)\rangle_{S_{\rm imp}} = \left\langle \sum_{i=1}^{m_F} \frac{\Delta(\tau,\tau_i^F-\tau_i'^F)}{\beta F(\tau_i^F-\tau_i'^F)} \right\rangle_{MC},$$
$$\langle b(\tau)b(0)\rangle_{S_{\rm imp}} = \left\langle \sum_{i=1}^{m_{K^*}} \frac{\Delta(\tau,\tau_i^{K^*}-\tau_i'^{K^*})}{\beta K^*(\tau_i^{K^*}-\tau_i'^{K^*})} \right\rangle_{MC},$$
$$\langle b(\tau)\rangle_{S_{\rm imp}} = \left\langle \sum_{i=1}^{m_{\phi^*}} \frac{\Delta(\tau,\tau_i^{\phi^*})}{\kappa\phi^*} \right\rangle_{MC},$$

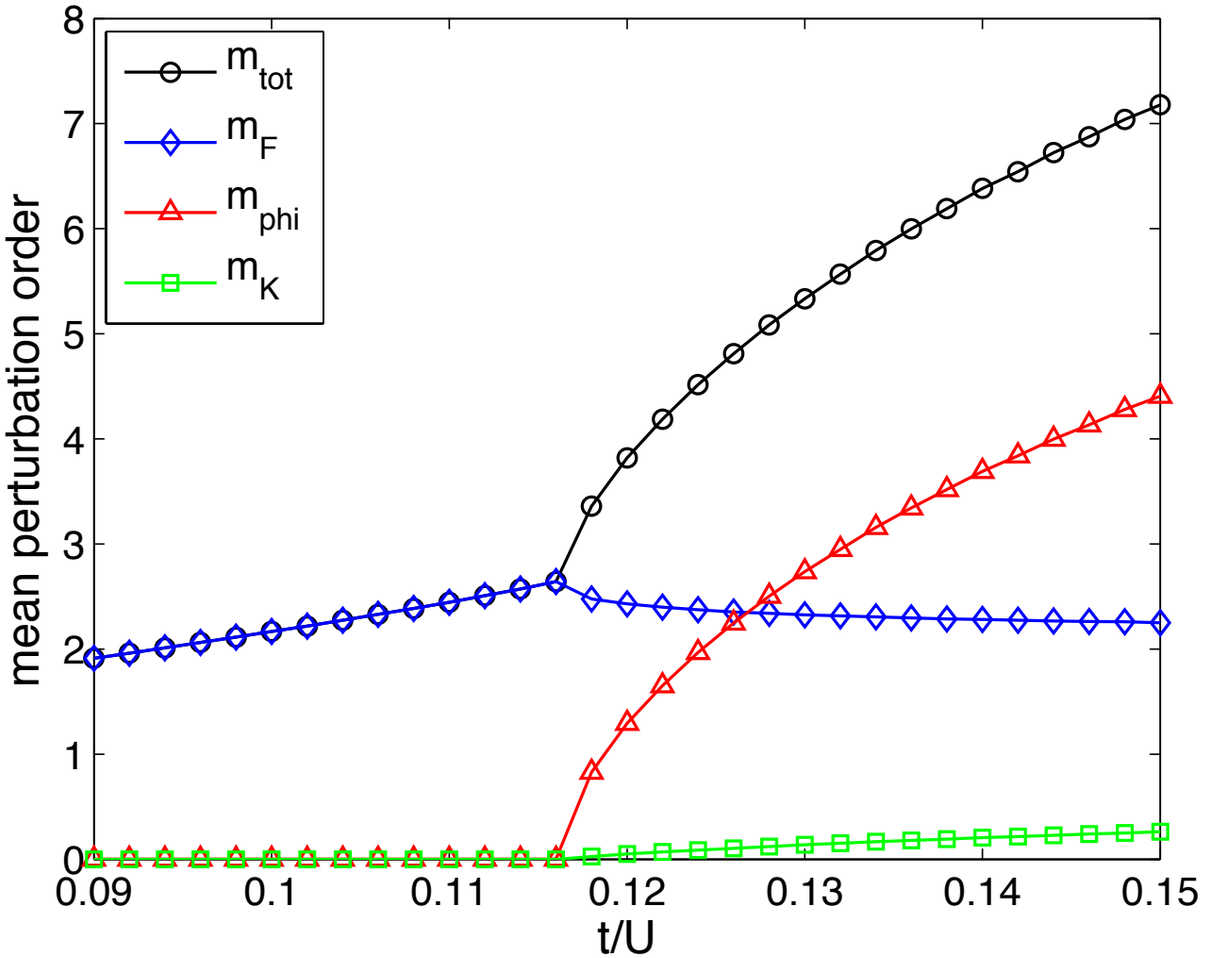
(perfect agreement with exact diagonalization)



$$\Delta(\tau,\tau') = \delta(\tau-\tau') \quad \tau \geq 0$$
$$= \delta(\tau-\tau'-\beta) \quad \tau < 0$$

perturbation orders

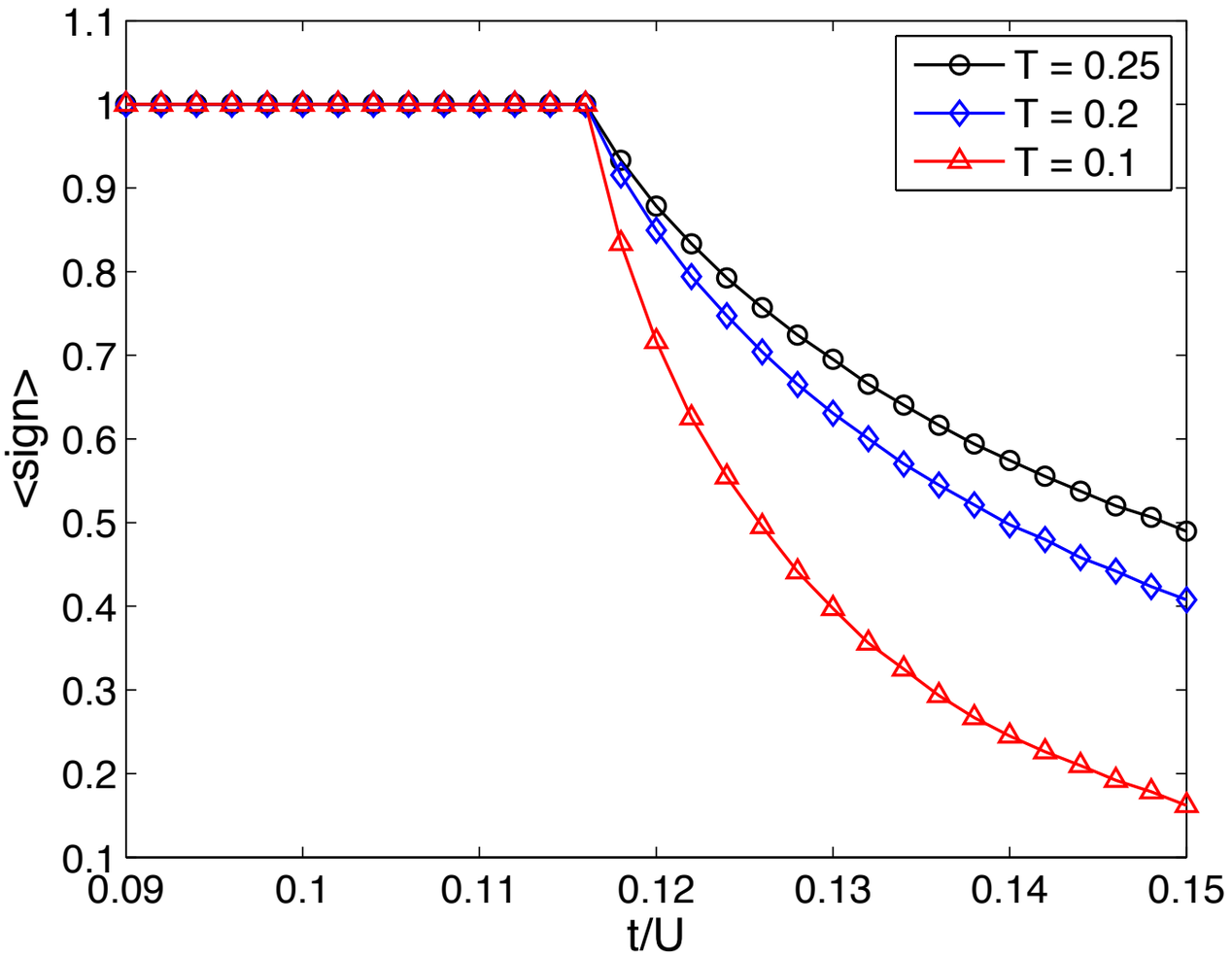
condensate and anomalous green functions only occur in the SF phase; transitions are continuous



$$n = 1, \beta = 5$$

sign

The anomalous green function introduces a sign *torture*
(in the superfluid phase only)

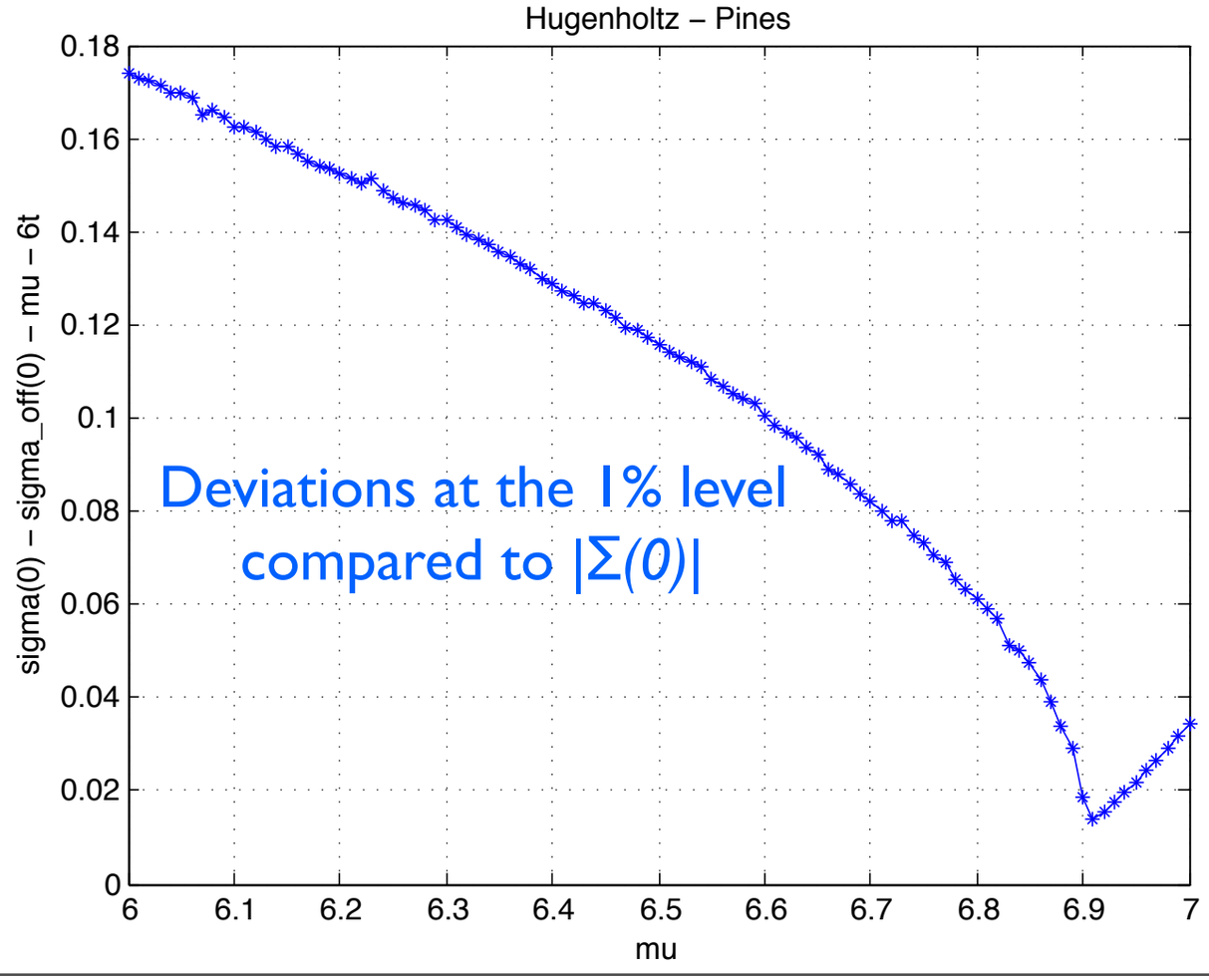


$$n = 1$$

on the Hugenholtz-Pines theorem

$$S_{\rm imp} = \int_0^\beta d\tau b^*_{\rm int}(\tau)(\partial_\tau - \mu) b_{\rm int}(\tau) + \frac{U}{2} n_{\rm int}(n_{\rm int}-1)$$
$$- zt\mathbf{\Phi}^\dagger_{\rm ext} \int_0^\beta d\tau \mathbf{b}_{\rm int}(\tau)$$
$$+ \int_0^\beta d\tau \int_0^\beta d\tau' (\mathbf{b}^\dagger_{\rm int}(\tau) - \mathbf{\Phi}_{\rm int}(\tau)) \mathbf{\Delta}(\tau-\tau') (\mathbf{b}_{\rm int}(\tau') - \mathbf{\Phi}_{\rm int}(\tau'))$$

- take only ϕ self-consistent: Hugenholtz-Pines is fulfilled up to shift 6t
- take both ϕ and Δ selfconsistenly : Hugenholtz-Pines is not fulfilled

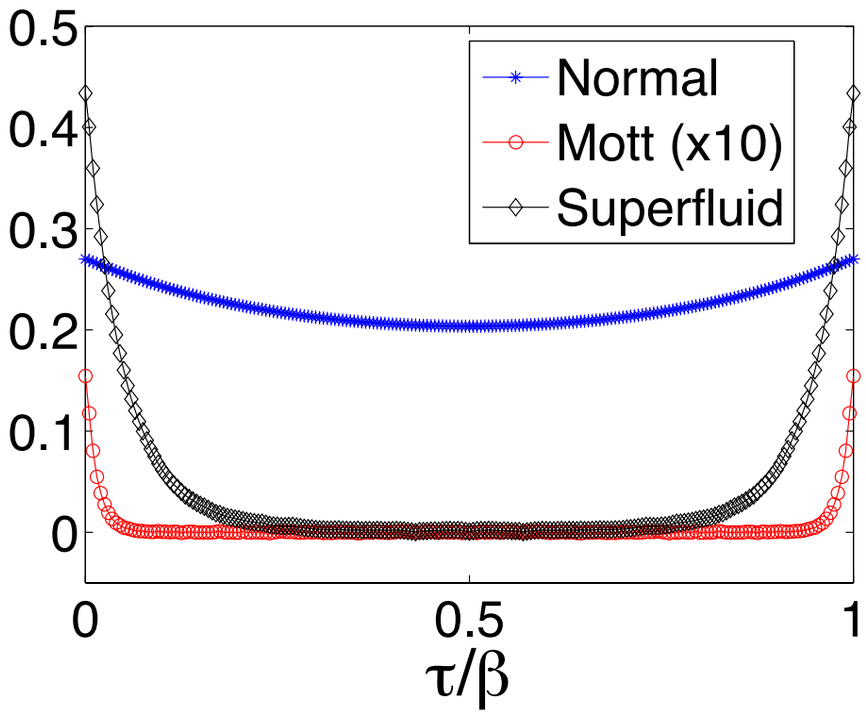


N. B. losing the equation of state is not uncommon for strong-coupling expansions

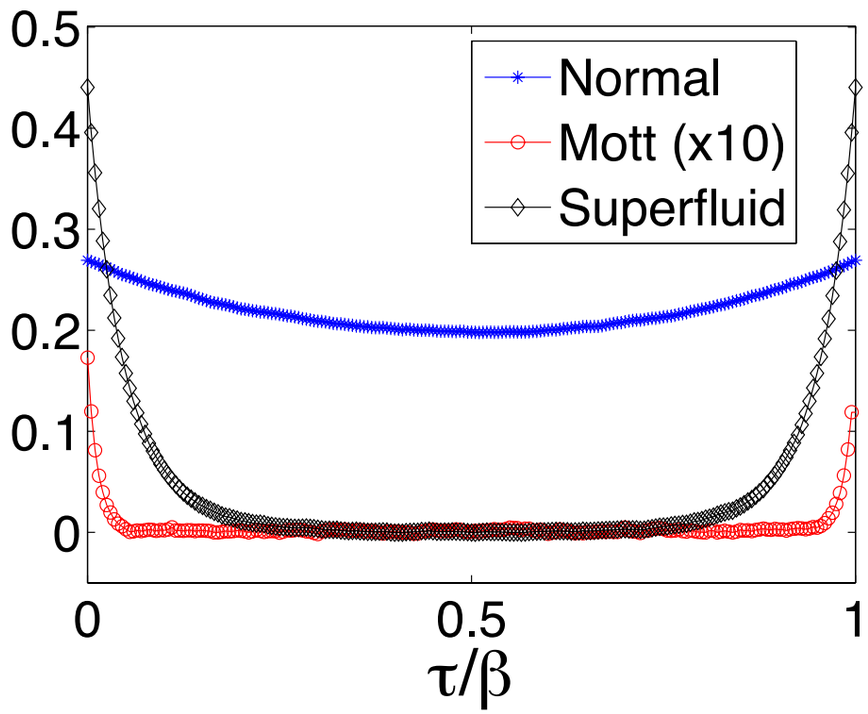
correlation functions

Density-density correlation function

BDMFT



QMC



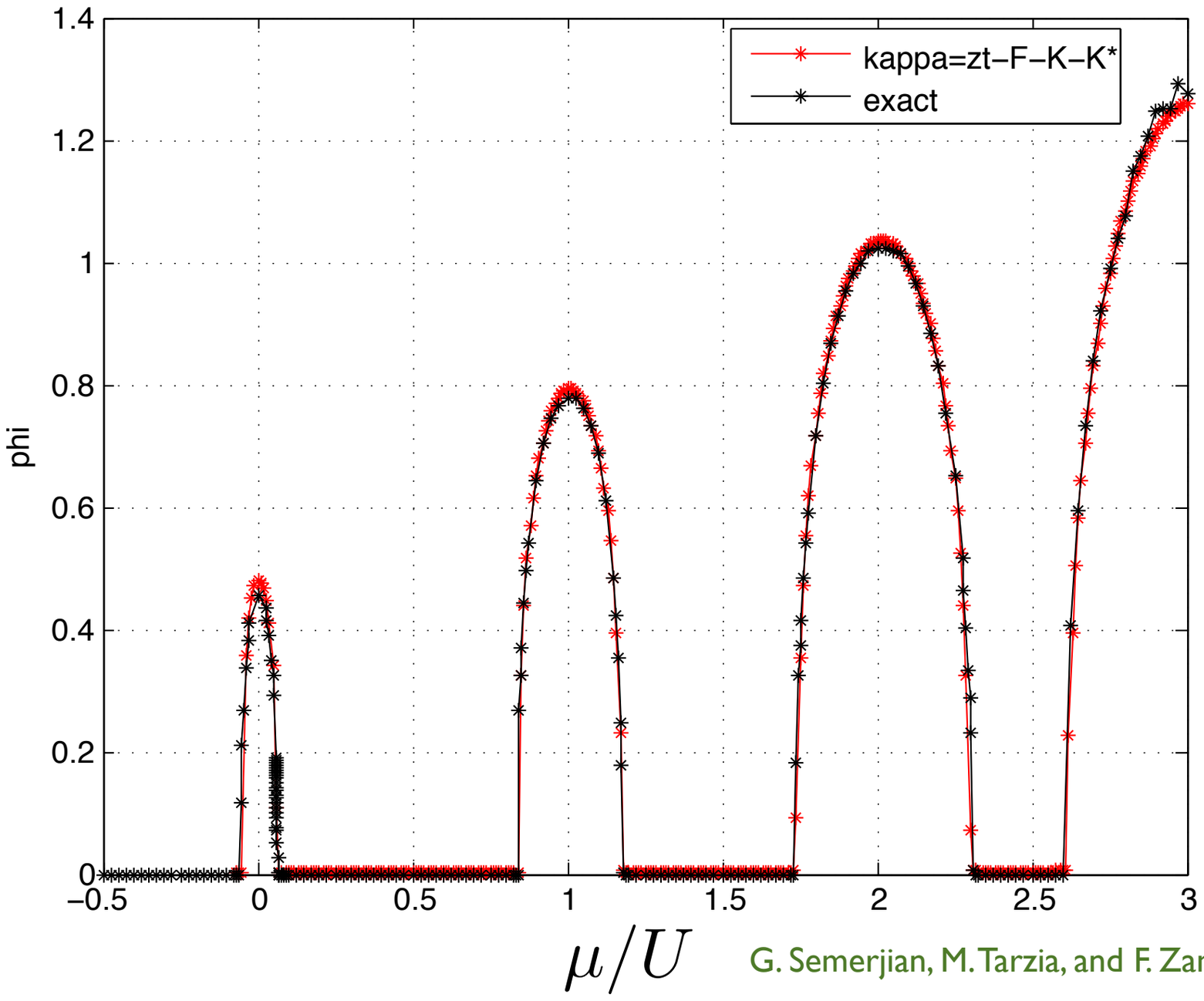
$(U,\ \mu)$	$n_{\text{B-DMFT}}$	n_{MC}	$\phi^2_{\text{B-DMFT}}$	ϕ^2_{MC}	sign
(20, 6.6)	0.99441(4)	0.99456(1)	0.5042(3)	0.486(2)	0.6373(1)
(24, 8.6)	0.99494(5)	0.995120(1)	0.3383(4)	0.316(1)	0.7836(1)
(26, 10)	1.00194(3)	1.001936(1)	0.2389(4)	0.2227(9)	0.8674(1)
(28, 11.3)	1.00252(3)	1.002598(4)	0.1087(5)	0.104(1)	0.9585(1)
(30, 13)	1.000403(5)	1.00041(4)	0	0	1
(32, 15)	1.000333(5)	1.000370(9)	0	0	1

$\beta = 1$

comparison with exact solution

Condensate density

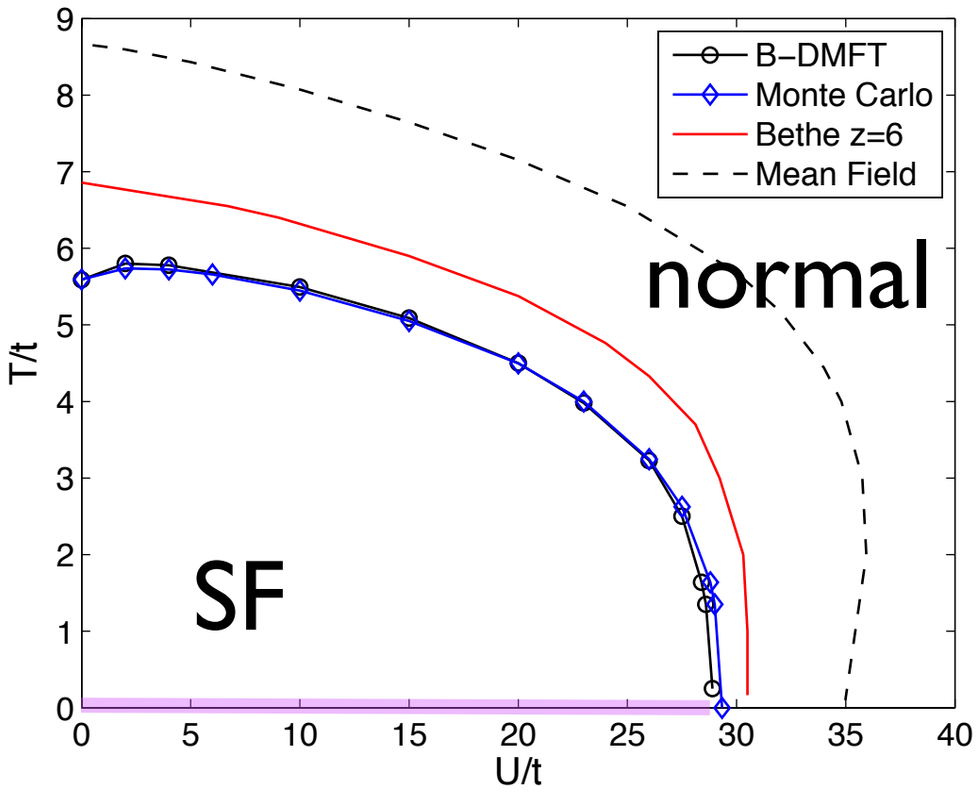
comparison between BDMFT and exact solution for tree lattice with z=4, β= 1



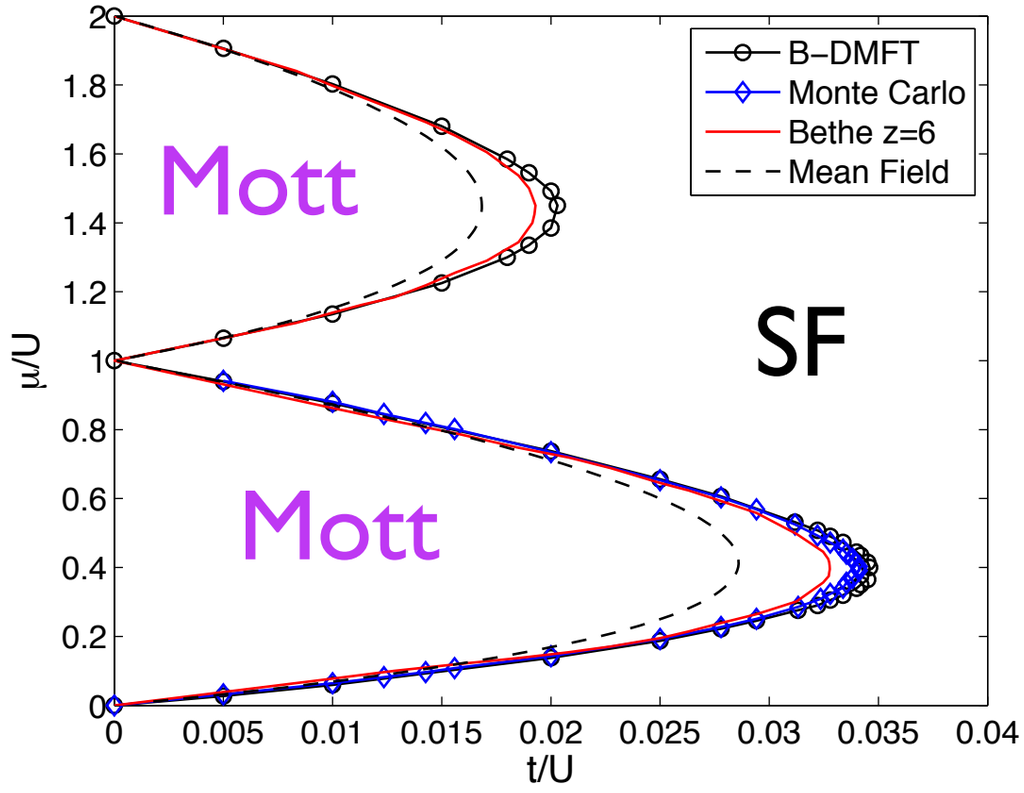
G. Semerjian, M. Tarzia, and F. Zamponi, Phys. Rev. B **80**, 014524 (2008).

3d phase diagram

finite temperature,
unity density

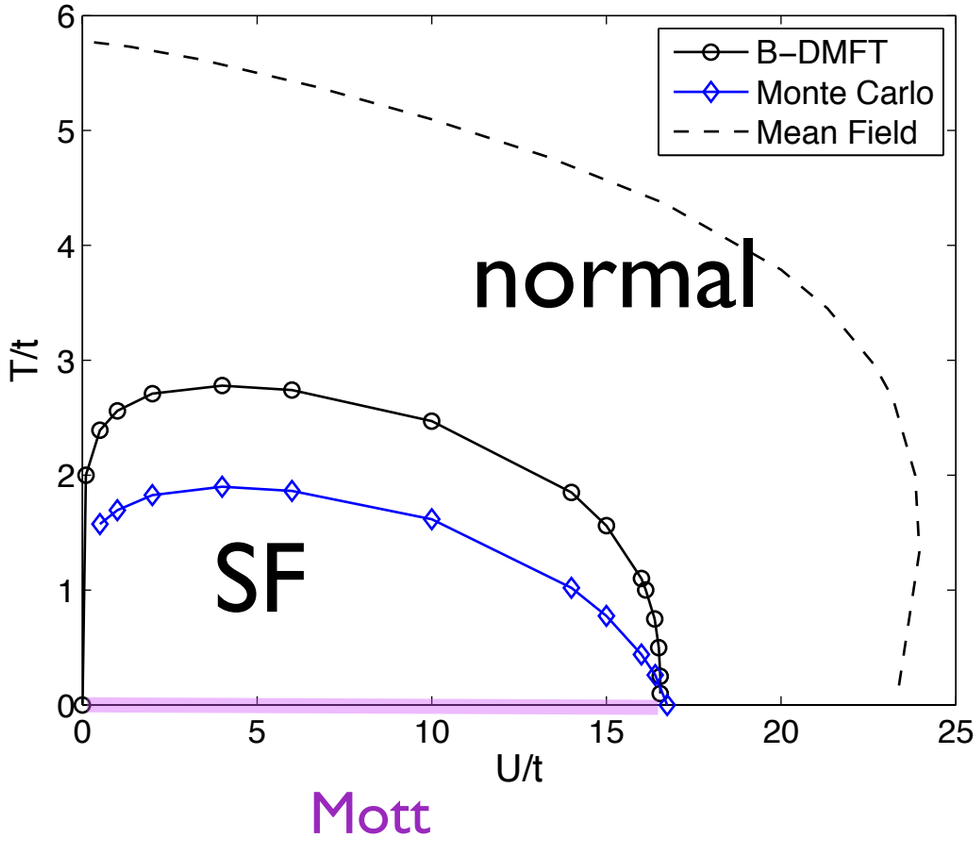


ground state

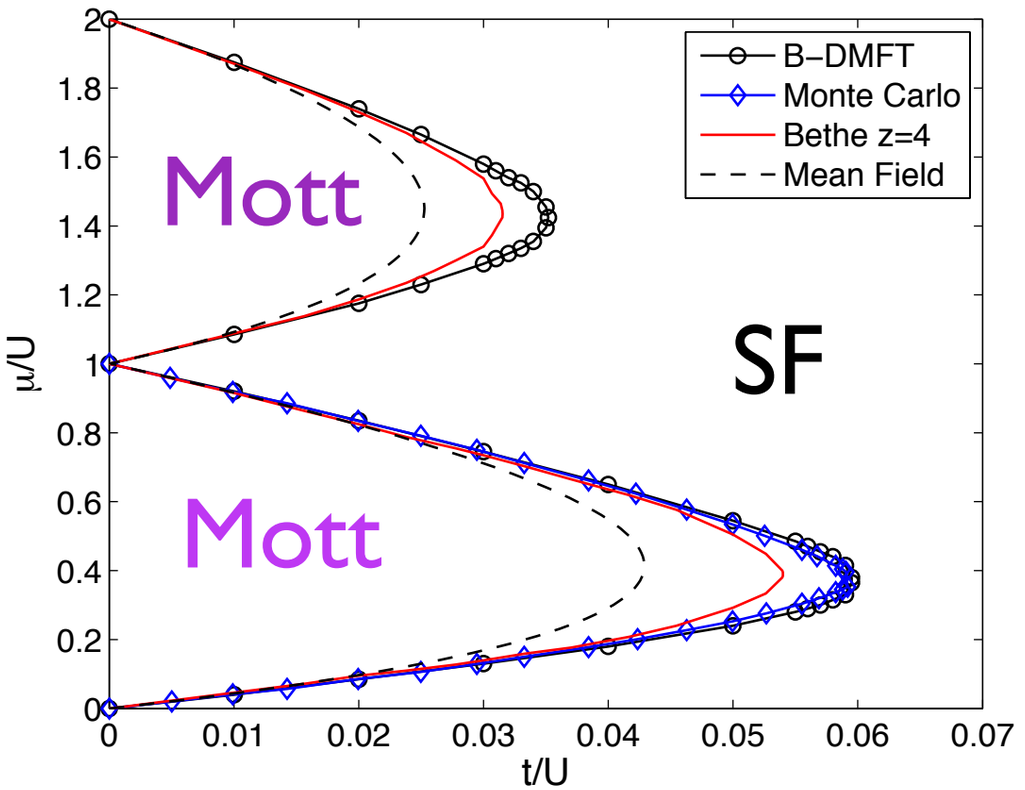


2d results

finite temperature, unity density

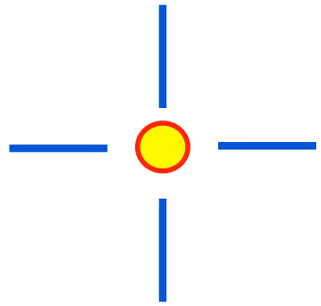


ground state



outlook

We have a mean-field theory with retardation effects, that builds in the broken symmetry and the one-loop correction correctly.
It can be seen as an *interpolation technique* between the non-interacting limit (Bogoliubov physics) and the atomic limit (Mott physics), which it reproduces correctly, and reduces to mean-field theory for infinite coordination number. It shows results for the Bose-Hubbard model with an accuracy that puzzles me.



BDMFT is a formalism under development. It may be a good starting point for undertaking further studies in otherwise hard/intractable systems:

- other impurity solvers?
- Bose-Fermi mixtures
- Bose-Bose mixtures and spinor bosons
- cluster-BDMFT
- bosonic impurity models (no bath)
- real-time dynamics beyond Gutzwiller?

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