Diagrammatic extensions of (E)DMFT: Dual boson

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Outline

- Motivation: Diagrammatic extensions of DMFT
- Overview
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  - Underlying idea
  - Dual fermion: convergence properties
- Collective excitations: dual boson approach
  - EDMFT
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  - Impurity Solver
  - Collective excitations: DMFT / EDMFT

Motivation

- include momentum dependence beyond DMFT
- quantum criticality
- long-range Coulomb interaction
- collective excitations
- Feasible / accurate many body approaches for real materials
- ...

Diagrammatic extensions of (extended) DMFT

- Diagrammatic extension of DMFT

  [H. Kusunose J. Phys. Soc. of Japan **75**, 054713 (2006)]

- Multiscale approach

  [C. Slezak, M. Jarrell, T. Maier, and J. Deisz, arXiv:0603421 (2006)]

- DΓA

  [A. Toschi, A. A. Katanin, and K. Held, Phys. Rev. B **75**, 045118 (2007)]

- Dual Fermion

  [A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B **77**, 033101 (2008)]

- Dual Boson

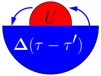
  [A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Ann. Phys. **327**, 1320 (2012)]

- One-particle irreducible approach

  [G. Rohringer, A. Toschi, H. Hafermann, K. Held, V. I. Anisimov, and A. A. Katanin,

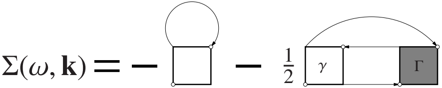
  Phys. Rev. B **88**, 115112 (2013)]

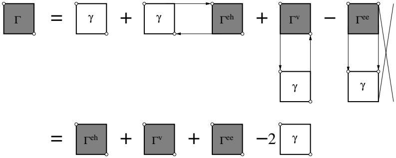
Diagrammatic extensions of DMFT: underlying idea



impurity model $\Longrightarrow \Sigma_\nu^{\text{imp}}$, **vertex** $\gamma_{\nu\nu'\omega}^{\text{imp}}$

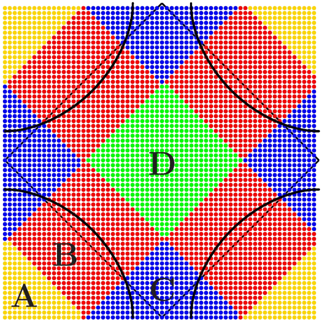
- utilize effective two-particle interaction of the impurity model





- include spatial correlations through diagrammatic corrections: second-order, ∼FLEX, ∼Parquet, diagrammatic MC (?) . . .

Complementarity to cluster approaches



Clusters

- Control parameter: cluster size
- Rigorous summation of all diagrams on the cluster
- limited cluster size, difficult to converge in practice

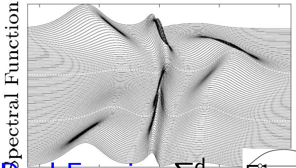
Diagrammatic extensions

- Large clusters
- Diagrams chosen on physical considerations
- Truncation of diagrammatic series and fermion interaction

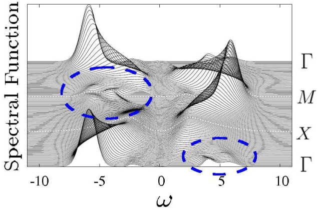
Illustration: dual fermion

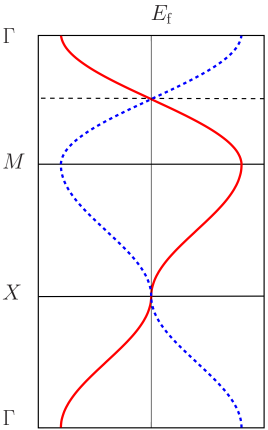
paramagnetic 2D Hubbard model, $U/t = 8$, $T/t = 0.235$

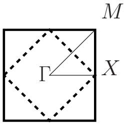
DMFT



Dual Fermion $\Sigma^{\mathrm{d}} =$ 







$\mathbf{Q} = (\pi, \pi)$

$\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}}$

- Captures short-range dynamical AF correlations
- Critical $U_c/t \sim 6.5$ in good agreement with cluster methods

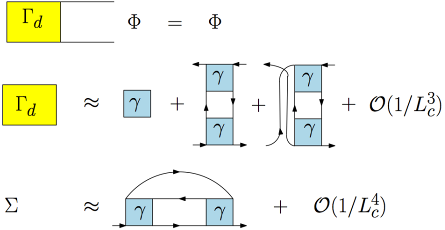
[S. Brener, HH, A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein PRB **77**, 195105 (2008)]

Convergence Properties I

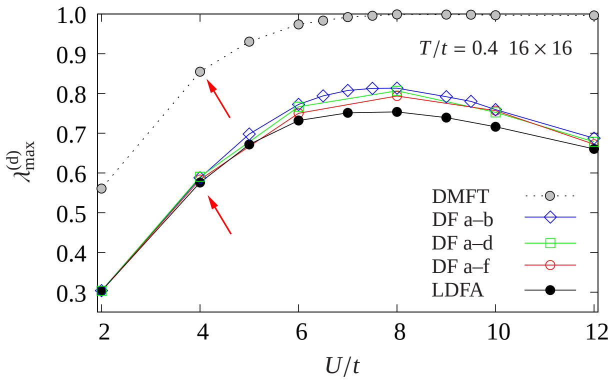
Small parameter?

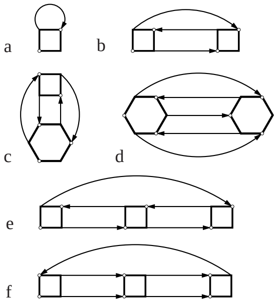
- weak coupling limit ($U \to 0$): $\gamma^{(4)} \sim U$, $\gamma^{(6)} \sim U^2$, ...
- strong coupling limit ($t \sim h_{\mathbf{k}} \to 0$); atomic limit ($\Delta \equiv 0$):

$$G^{\mathrm{d}\ 0}_{\omega}(\mathbf{k}) = g_\omega \left[g_\omega + (\Delta - h_{\mathbf{k}})^{-1}\right]^{-1} g_\omega \approx g_\omega\, h_{\mathbf{k}}\, g_\omega$$

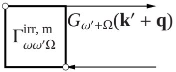


Convergence Properties II





$$-\frac{T}{N}\sum_{\omega'\mathbf{k}'}\Gamma^{\text{irr, m}}_{\omega\omega'\Omega=0}\, G_{\omega'}(\mathbf{k})G_{\omega'}(\mathbf{k}+\mathbf{Q})\,\phi_{\omega'} = \lambda\phi_{\omega'}$$



DF: $\Gamma^{\text{irr}} = \gamma^{(4)}$, $G = G^{\text{d}}$ DMFT: $\Gamma^{\text{irr}} = \gamma^{\text{irr}}_{\text{imp}}$, $G = G^{\text{DMFT}}$

[HH, G. Li, A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, H. Monien, Phys. Rev. Lett. **102**, 206401 (2009)]

Extended Hubbard model Hamiltonian

$$H = -\tilde{t}\sum_{\mathbf{r}\delta\sigma}\left(c^{\dagger}_{\mathbf{r}\sigma}c_{\mathbf{r}-\delta\sigma} + c^{\dagger}_{\mathbf{r}-\delta\sigma}c_{\mathbf{r}\sigma}\right) + U\sum_{\mathbf{r}} n_{\mathbf{r}\uparrow}n_{\mathbf{r}\downarrow} + \frac{1}{2}\sum_{\mathbf{r}\mathbf{r}'} V(\mathbf{r}-\mathbf{r}')n_{\mathbf{r}}n_{\mathbf{r}'}.$$

$\mathbf{r}$: <u>discrete</u> lattice site positions; half bandwidth $D = 1$

- $V_{\mathbf{q}} = 0$ local interaction $\rightarrow$ Hubbard model (2D)
- $V_{\mathbf{q}} = \frac{V}{q^2}$, (screened) Coulomb interaction (3D)
- $V_{\mathbf{q}} = 2V(\cos q_x + \cos q_y)$, nearest-neighbor interaction (2D)

Extended dynamical mean-field theory (EDMFT)

- Treatment of models with long-range interaction $V_{\mathbf{q}}$
- Mapping to impurity model with retarded interaction W_ω

$$S_{\text{imp}}[c^*, c] = -\sum_{\nu\sigma} c^*_{\nu\sigma}[\imath\nu + \mu - \Delta_{\nu\sigma}]c_{\nu\sigma}$$
$$+ U\sum_{\omega} n_{\omega\uparrow}n_{-\omega\downarrow} + \frac{1}{2}\sum_{\omega} n_\omega W_\omega n_{-\omega}.$$

$$G^{-1}_\nu(\mathbf{k}) = (g^{\text{imp}}_\nu)^{-1} + \Delta_\nu - \epsilon_{\mathbf{k}}$$
$$X^{-1}_\omega(\mathbf{q}) = (\chi^{\text{imp}}_\omega)^{-1} + W_\omega - V_{\mathbf{q}}$$

Self-consistency

$$g^{\text{imp}}_\nu = \frac{1}{N}\sum_{\mathbf{k}} G_\nu(\mathbf{k})$$

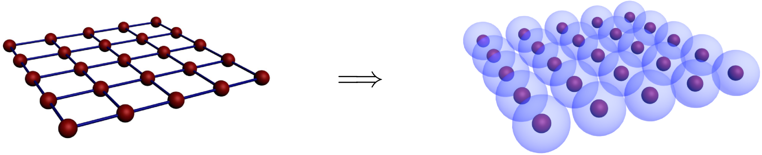
$$\chi^{\text{imp}}_\omega = \frac{1}{N}\sum_{\mathbf{q}} X_\omega(\mathbf{q})$$

[Q. Si and J. L. Smith, Phys. Rev. Lett. **77**, 3391 (1996)] [H. Kajueter, Ph.D. thesis, Rutgers University (1996)]
[J. L. Smith and Q. Si, Phys. Rev. B **61**, 5184 (2000)] [R. Chitra and G. Kotliar, Phys. Rev. B **63**, 115110 (2001)]

dual bosons: basic idea

$$S_{\text{lat}}[c^*, c] = -\sum_{i\nu\sigma} c^*_{i\nu\sigma}[\imath\nu + \mu]c_{i\nu\sigma} + U\sum_{\mathbf{q}\omega} n_{\mathbf{q}\omega\uparrow}n_{-\mathbf{q},-\omega\downarrow}$$
$$+\sum_{\mathbf{k}\nu\sigma} \varepsilon_{\mathbf{k}} c^*_{\mathbf{k}\nu\sigma}c_{\mathbf{k}\nu\sigma} + \frac{1}{2}\sum_{\mathbf{q}\omega} V_{\mathbf{q}} n_{\mathbf{q}\omega} n_{-\mathbf{q}-\omega}.$$

Introduce impurity problem at each lattice site



$$S_{\text{lat}}[c^*, c] = \sum_i S_{\text{imp}}[c^*_{\nu i\sigma}, c_{\nu i\sigma}] - \sum_{\nu\mathbf{k}\sigma} c^*_{\nu\mathbf{k}\sigma}(\Delta_\nu - \epsilon_{\mathbf{k}})c_{\nu\mathbf{k}\sigma}$$
$$-\sum_{\omega\mathbf{q}} n_{\omega\mathbf{q}}(W_\omega - V_{\mathbf{q}})n_{\omega\mathbf{q}}$$

decouple non-local terms through Hubbard-Stratonovich transformations, integrate out original fermions

[A.N. Rubtsov, M.I. Katsnelson, A.I. Lichtenstein, Ann. Phys. **327**, 1320 (2012)]

Transformation to Dual Fermions

$$e^{c^*_{\nu\mathbf{k}\sigma}(\Delta_\nu-\epsilon_\mathbf{k})c_{\nu\mathbf{k}\sigma}} = \det\left[g_\nu^{-1}(\Delta_\nu-\epsilon_\mathbf{k})g_\nu^{-1}\right]^{-1}\times$$

$$\times\int\mathcal{D}[f,f^*]e^{-f^*_{\nu\mathbf{k}\sigma}g_\nu^{-1}(\Delta_\nu-\epsilon_\mathbf{k})g_\nu^{-1}f_{\nu\mathbf{k}\sigma}-f^*_{\nu\mathbf{k}\sigma}g_\nu^{-1}c-c^*g_\nu^{-1}f_{\nu\mathbf{k}\sigma}}$$

$$e^{\frac{1}{2}n^*_{\omega\mathbf{q}}(W_\omega-V_\mathbf{q})n_{\omega\mathbf{q}}} = \det\left[\chi_\omega^{-1}(W_\omega-V_\mathbf{q})\chi_\omega^{-1}\right]^{-\frac{1}{2}}\times$$

$$\times\int\frac{\mathcal{D}[\phi]}{\sqrt{(2\pi)^N}}e^{-\phi_{\omega\mathbf{q}}\chi_\omega^{-1}(W_\omega-V_\mathbf{q})\chi_\omega^{-1}\phi_{\omega\mathbf{q}}-\phi_{\omega\mathbf{q}}\chi_\omega^{-1}n_{\omega\mathbf{q}}-n_{\omega\mathbf{q}}\chi_\omega^{-1}\phi_{\omega\mathbf{q}}}$$

$\rightarrow$ dual action

$$S[f^*,f] = \sum_{\nu\mathbf{k}\sigma}f^*_{\nu\mathbf{k}\sigma}[G^{\mathrm{d}\,0}_\nu(\mathbf{k})]^{-1}f_{\nu\mathbf{k}\sigma}+\sum_i V[f^*_i,f_i;\phi_i]$$

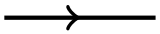
$$V[f^*,f;\phi] = -\frac{1}{4}\gamma_{1234}f_1f_2^*f_3f_4^*+\lambda_{123}f_1f_2^*\phi_3+\ldots$$

$$G^{\mathrm{d}\,0}_\nu(\mathbf{k}) = \left[g_\nu^{-1}+(\Delta_\nu-h_\mathbf{k})\right]^{-1}-g_\nu$$

$$X^{\mathrm{d}\,0}_\omega(\mathbf{k}) = \left[\chi_\omega^{-1}+(W_\omega-V_\mathbf{q})\right]^{-1}-\chi_\omega$$

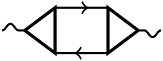
Dual perturbation theory

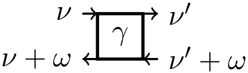
Evaluate fermionic and bosonic self-energies $\tilde{\Sigma}$, $\tilde{\Pi}$ in dual perturbation theory



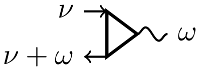
(a) $\tilde{G}^{(0)}_{\mathbf{k}\nu}$

(b) $\tilde{X}^{(0)}_{\mathbf{q}\omega}$





(c) $\gamma^{\text{imp}}_{\nu\nu'\omega}$



(d) $\lambda^{\text{imp}}_{\nu\omega}$

Polarization corrections

$\tilde{\Sigma} = \tilde{\Pi} = 0$ corresponds to (extended) DMFT:

$$G^{-1}_{\mathbf{k}\nu} = g^{-1}_{\nu}(1 + \tilde{\Sigma}_{\mathbf{k}\nu} g_{\nu})^{-1} + \Delta_{\nu} - \epsilon_{\mathbf{k}}$$

$$X^{-1}_{\mathbf{q}\omega} = \chi^{-1}_{\omega}(1 + \tilde{\Pi}_{\mathbf{q}\omega} \chi_{\omega})^{-1} + W_{\omega} - V_{\mathbf{q}}$$

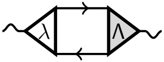
Define physical polarization:

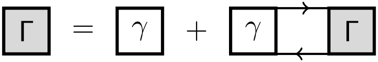
$$X^{-1}_{\mathbf{q}\omega} = -\Pi^{-1}_{\mathbf{q}\omega} - V_{\mathbf{q}}$$

$\tilde{\Pi}$ generates polarization corrections to EDMFT polarization

$$\Pi^{-1}_{\mathbf{q}\omega} = -\chi_{\omega}(1 + \tilde{\Pi}_{\mathbf{q}\omega} \chi_{\omega})^{-1} + W_{\omega}$$

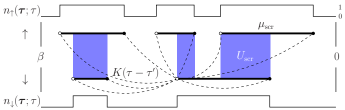
This talk: $\tilde{\Sigma} = 0$,

$\tilde{\Pi} =$ 



Impurity solver

Hybridization expansion CTQMC with retarded interaction U_ω and improved estimators



$$Z = Z_{\rm at} \sum_{k=0}^{\infty} \int d\boldsymbol{\tau}\, w_{\rm hyb}(\boldsymbol{\tau}) w_{\rm at}(\boldsymbol{\tau}) w_{\rm ret}(\boldsymbol{\tau})$$

$$w_{\rm at}(\boldsymbol{\tau}) = e^{-\frac{1}{2}\sum_{ij} U_{ij} l_{ij}} e^{\mu \sum_i l_{ii}}$$

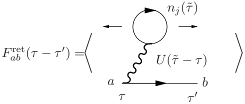
$$w_{\rm ret}(\boldsymbol{\tau}) = e^{\frac{1}{2}\sum_{ij}\sum_{2k_{i,j}\geq\alpha_i,\alpha_j>0}^{\alpha_i\neq\alpha_j} s_{\alpha_i} s_{\alpha_j} K(\tau_{\alpha_i}-\tau_{\alpha_j})} e^{2K'(0^+)\sum_{ij}^{i\neq j} l_{ij} + K'(0^+)\sum_i l_{ii}},$$

$$K''(\tau) = U(\tau), \qquad K(0) = K(\beta) = 0$$

[P. Werner et al., PRL **97**, 076405 (2006)] [P. Werner et al., PRL **104**, 146401 (2010)]

Improved estimators

$$\Sigma_a(i\omega) = \frac{F_a(i\omega)}{G_a(i\omega)}; \qquad F = F^{\text{st}} + F^{\text{ret}}$$

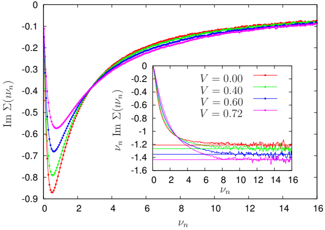


$$F_a^{\text{st}}(\tau-\tau') = -\sum_j \langle n_j(\tau) U_{ja} c_a(\tau) c_a^*(\tau') \rangle$$

$$F_a^{\text{ret}}(\tau-\tau') = -\int_0^\beta d\tilde\tau \sum_i \langle n_i(\tilde\tau) U_{\text{ret}}(\tilde\tau-\tau) c_a(\tau) c_a^*(\tau') \rangle \,.$$

$$\sum_j \int_0^\beta d\tilde\tau\, n_j(\tilde\tau) U_{\text{ret}}(\tilde\tau - \tau_\alpha^e)$$

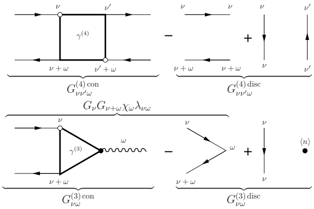
$$= -2K'(0^+) - \sum_j \sum_{\beta_j} s_{\beta_j} K'(\tau_{\beta_j} - \tau_\alpha^e)$$



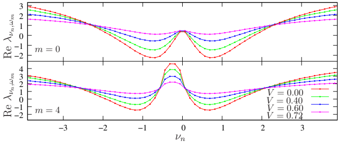
[HH, Phys. Rev. B **89**, 235128 (2014)]

Improved estimators for vertex

$$G^{(3),\text{con}}_{ab}(\imath\nu,\imath\omega) = \sum_i G_a(i\nu) F^{(3)}_{ab}(\imath\nu,\imath\omega) - \sum_i F'_a(\imath\nu) G^{(3)}_{ab}(\imath\nu,\imath\omega)$$



$$\lambda_a(\imath\nu,\imath\omega) = \frac{1}{\chi(\imath\omega)}\left(\sum_b G_a^{-1}(\imath\nu) G_a^{-1}(\imath\nu+\imath\omega) \times G^{(3),\text{con}}_{ab}(\imath\nu,\imath\omega) - 1\right)$$

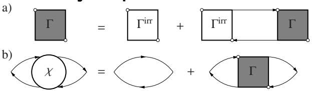


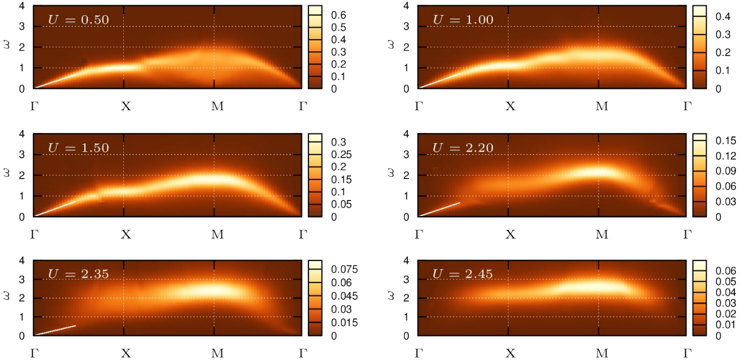
[HH, Phys. Rev. B **89**, 235128 (2014)]

Hubbard model (2D)

Collective charge excitations: DMFT ($V_{\mathbf{q}} = 0$)

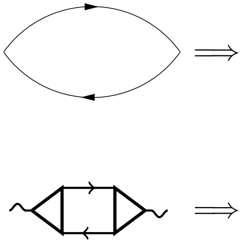
- Exactly equivalent to DMFT susceptibility

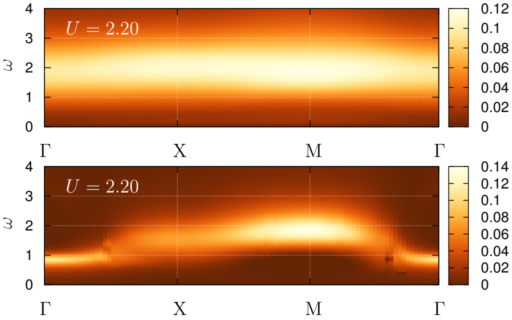




- zero sound mode in correlated metallic state

Simpler approximations





- approximations violate Ward identity (continuity equation)

$$q^F_\mu \Gamma_\mu(k, q) = G^{-1}(k) - G^{-1}(k+q)$$

- improper treatment of vertex corrections leads to qualitatively wrong results

DMFT susceptibility

DMFT is conserving!
Luttinger-Ward functional

$$\Phi[G_{i'j'}] = \sum_{i'} \Phi[G_{i'i'}] = \sum_{i'} \phi^{\text{imp}}[G_{i'i'}]$$

$$\Sigma_{ij} = \frac{\delta \Phi[G_{i'j'}]}{\delta G_{ji}} = \frac{\delta \phi[G_{i'i'}]}{\delta G_{ii}} \delta_{ji}$$

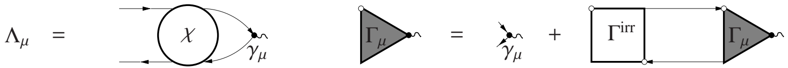
$$\Gamma^{\text{irr}}_{ijkl} = \frac{\delta^2 \Phi[G_{i'j'}]}{\delta G_{ji} \delta G_{lk}} = \frac{\delta^2 \phi[G_{l'l'}]}{\delta G_{ll}^2} \delta_{li} \delta_{lj} \delta_{lk}$$

$$\Sigma = \Sigma^{\text{imp}}, \qquad \Gamma^{\text{irr}} = \Gamma^{\text{irr,imp}}$$

[G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961)][G. Baym, Phys. Rev. **127**, 1391 (1962)]

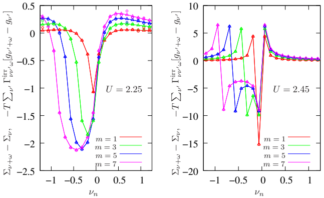
Ward identity

$$\Gamma_{\mu;\nu,\omega}(\mathbf{k},\mathbf{q}) = \gamma_\mu(\mathbf{k},\mathbf{q}) - T\sum_{\nu'\mathbf{k}'}\Gamma^{\text{irr}}_{\nu\nu'\omega}G_{\nu'\sigma'}(\mathbf{k}')G_{\nu'+\omega}(\mathbf{k}'+\mathbf{q})\Gamma_{\mu;\nu',\omega}(\mathbf{k}',\mathbf{q}).$$



$$q^F_\mu\Gamma_{\mu;\nu}(\mathbf{k},\mathbf{q}) = q^F_\mu\gamma_\mu(\mathbf{k},\mathbf{q}) - T\sum_{\nu'\mathbf{k}'}\Gamma^{\text{irr}}_{\nu\nu'\omega}$$

$$\times\, G_{\nu'}(\mathbf{k}')G_{\nu'+\omega}(\mathbf{k}'+\mathbf{q})[q^F_\mu\Gamma_{\mu;\nu'}(\mathbf{k}',\mathbf{q})]$$



$$\frac{\Sigma_{\nu+\omega}-\Sigma_\nu}{\omega} = -T\sum_{\nu'}\Gamma^{\text{irr}}_{\nu\nu'\omega}\frac{[g_{\nu'+\omega}-g_{\nu'}]}{\omega}$$

Collective charge excitations: EDMFT ($V_{\mathbf{q}} = V/q^2$, 3D)

EDMFT:

$$X_\omega(\mathbf{q}) = \frac{1}{[(\chi_\omega^{\text{imp}})^{-1} + W_\omega] - V_{\mathbf{q}}}$$

$$1 + V\Pi_{\omega(q)}/q^2 = 0$$

$$\Pi_\omega \sim 1/\omega^\alpha \Longrightarrow \omega \sim 1/q^{2/\alpha}$$

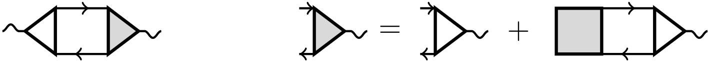
RPA:

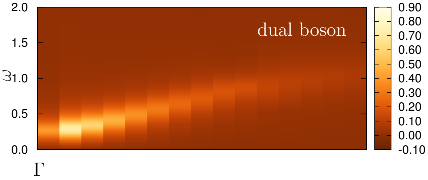
$$X_\omega(\mathbf{q}) = \frac{1}{-\Pi_\omega^{\text{RPA}}(\mathbf{q}) - V_{\mathbf{q}}}$$

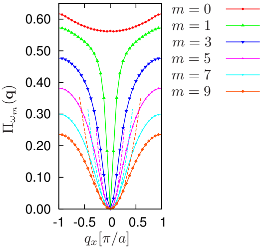
$$1 + V\Pi_{\omega(q)}(\mathbf{q})/q^2 = 0$$

$$\Pi_\omega^{\text{RPA}}(\mathbf{q}) = -\chi_\omega^0(\mathbf{q}) \sim g\, q^2 f(\omega)$$

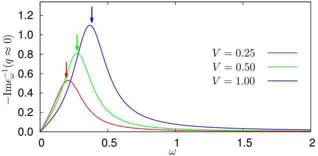
Collective charge excitations: $(V_{\mathbf{q}} = V/q^2$, 3D$)$







dual boson polarization
$\Pi_\omega(\mathbf{q}) \sim q^2 \ (\omega > 0)$

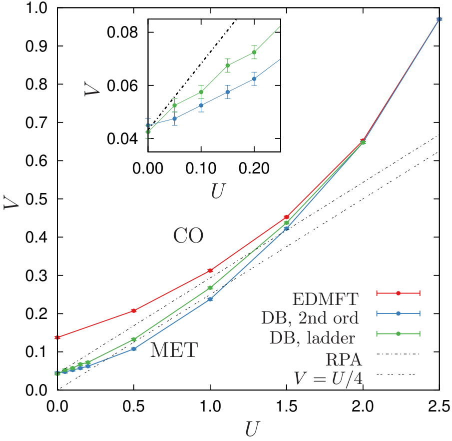


plasma frequency:

$$\omega_p^2 = e^2 a^2 t V \sum_{\mathbf{k}\sigma} 2\cos(k_z a) \langle n_{\mathbf{k}\sigma} \rangle$$

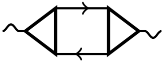
Extended Hubbard model: $U - V$ phase diagram (2D)

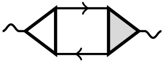
transition to charge-ordered (CO) insulator



divergence of $X_{\mathbf{q}\omega}$ at $\mathbf{q} = (\pi, \pi)$, $\omega = 0$

dual boson diagrams:





- large corrections to EDMFT even for small U
- RPA is reproduced non-trivially for $U \to 0$!

Summary

- DMFT susceptibility provides conserving description of the collective excitations of strongly correlated electrons
- dual boson approach yields conserving description of collective charge excitations in correlated systems
  (zero sound / plasmons)
- *non-local* vertex corrections are *essential*
  to fulfill charge conservation
- frequency dependent self-energy requires
  frequency dependent irreducible vertex

Thank you for your attention !