Collective charge excitations of strongly correlated electrons, vertex corrections and gauge invariance

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Collaborators

In collaboration with

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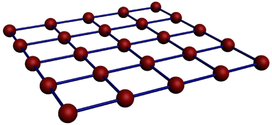
- Erik van Loon (University of Nijmegen, The Netherlands)
- Alexander Lichtenstein (University of Hamburg, Germany)
- Olivier Parcollet (CEA, Saclay, France)
- Alexey Rubtsov (Moscow State University, Russia)

Outline

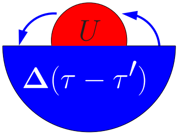
- Motivation: Diagrammatic extensions of DMFT
- Short-range interaction: Hubbard model
  - RPA
  - DMFT
- Charge conservation, vertex corrections & Ward identity
- Long-range forces: extended Hubbard model
  - RPA
  - Extended DMFT
  - Dual boson approach
- Role of vertex corrections in dual boson

Recollection of DMFT

Mapping to impurity problem



$\Longrightarrow$



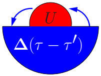
$$G_\nu(\mathbf{k}) = \frac{1}{\imath\nu + \mu - \epsilon_{\mathbf{k}} - \Sigma_\nu^{\text{imp}}}$$

Self-consistency condition

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

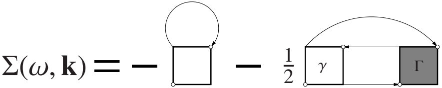
[A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)]

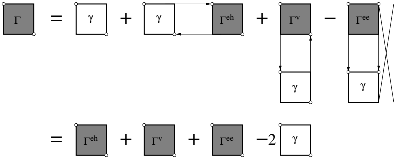
Diagrammatic extensions of (extended) DMFT



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

- Include spatial correlations through diagrammatic corrections: second-order, FLEX, Parquet, . . .





- Examples: DΓA, 1PI, dual fermion, dual boson approach

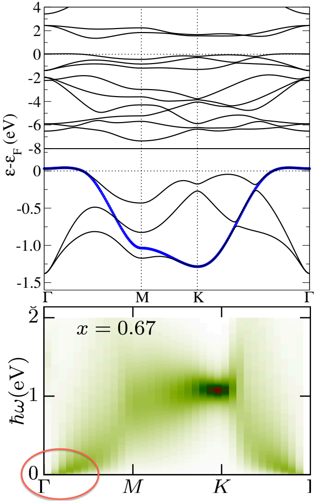
[A. Toschi, A. A. Katanin, and K. Held, PRB **75**, 045118 (2007)]

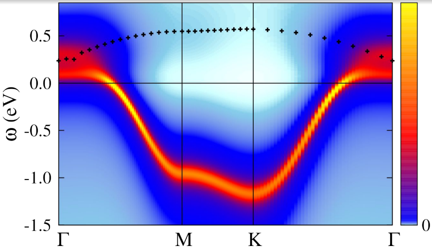
[A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, PRB **77**, 033101 (2008)]

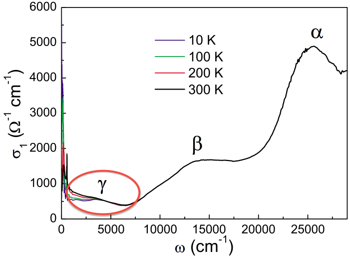
[A.N. Rubtsov, M.I. Katsnelson, A.I. Lichtenstein, Ann. Phys. **327**, 1320 (2012)]

[G. Rohringer, A. Toschi, H. Hafermann, K. Held, V. I. Anisimov, and A. A. Katanin, PRB **88**, 115112 (2013)]

Example: Spinpolarons in Na_xCoO_2





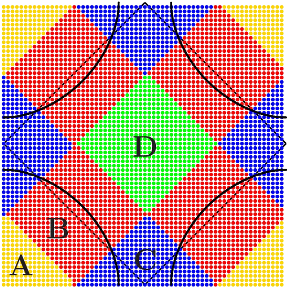


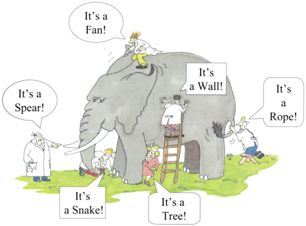
[L. Boehnke, F. Lechermann, Phys. Rev. B **85**, 115128 (2012)]

[A. Wilhelm, F. Lechermann, HH, M. I. Katsnelson, A .I. Lichtenstein, arXiv:1408.2152 (2014)]

[N. L. Wang, P. Zheng, D. Wu, and Y. C. Ma, T. Xiang, R.Y. Jin and D. Mandrus, PRL **93**, 237007 (2004)]

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
- Ambiguous interpolation

Diagrammatic extensions

- Large clusters
- No sign problem
- Diagrams summed perturbatively
- Truncation of fermion-fermion interaction

Model

Extended Hubbard model Hamiltonian

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

$\mathbf{r}$: discrete 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)
- $V_{\mathbf{q}} = \frac{V}{q}$, (screened) Coulomb interaction (2D)
- $V_{\mathbf{q}} = 2V(\cos q_x + \cos q_y)$, nearest-neighbor interaction (2D)

Model

Extended Hubbard model Hamiltonian

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

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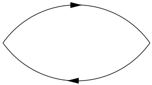
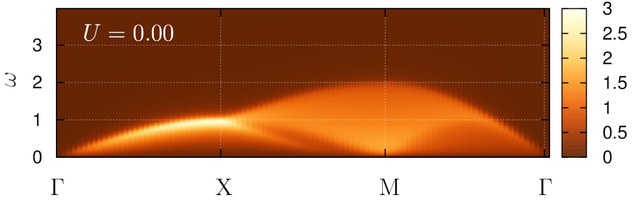
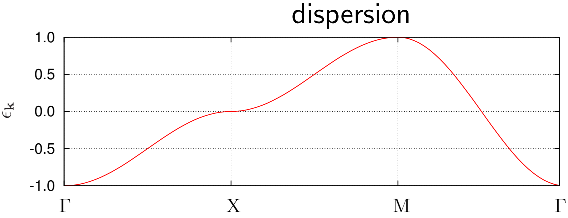
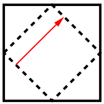
Noninteracting case: $\chi^0_\omega(\mathbf{q}) = -\frac{T}{N}\sum_{\mathbf{k}\nu\sigma} G_{\nu+\omega}(\mathbf{k}+\mathbf{q})G_\nu(\mathbf{k})$

$\chi^0_\omega(\mathbf{q}) =$ 



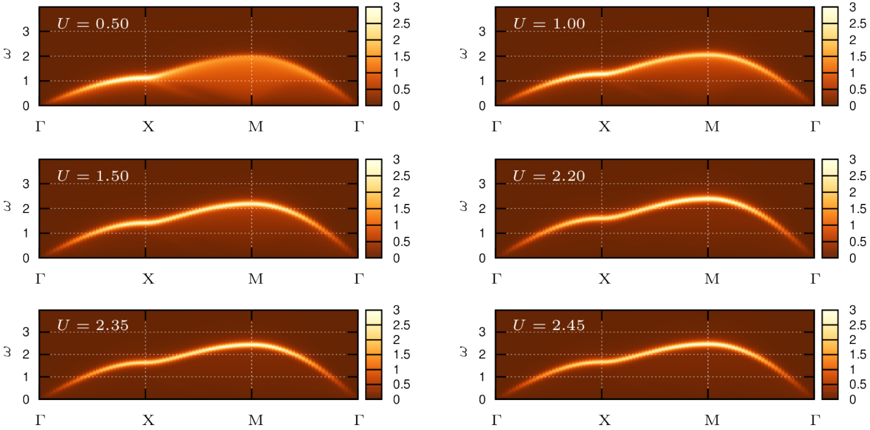




$\mathbf{Q} = (\pi, \pi)$

Hubbard model ($V_{\mathbf{q}} = 0$)

Random phase approximation ($T = 0.02$)



- Zero sound mode for $q \to 0$
- RPA does not capture Mott physics

Hubbard model ($V_{\mathbf{q}} = 0$)

Random phase approximation

$$\chi_\omega(\mathbf{q}) = -\Pi_\omega(\mathbf{q}) + \Pi_\omega(\mathbf{q}) U \Pi_\omega(\mathbf{q}) - \ldots = \frac{-\Pi_{\omega(\mathbf{q})}}{1 + U\Pi_\omega(\mathbf{q})}$$

$$\Pi_\omega^{\mathrm{RPA}}(\mathbf{q}) = -\chi_\omega^0(\mathbf{q})$$

Polarization

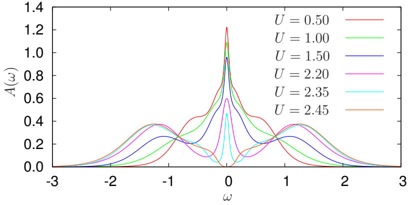
$$\Pi_\omega^{\mathrm{RPA}}(\mathbf{q}) = -\sum_{\mathbf{k}\sigma} \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{k}+\mathbf{q}})}{\imath\omega + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}} \overset{q\to 0}{\sim} \frac{q^2}{(\imath\omega)^2}$$

Dispersion of collective mode:

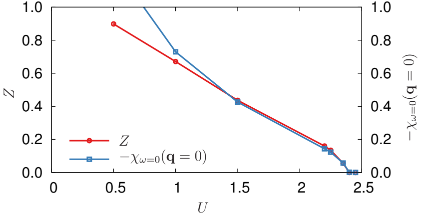
$$1 + U\Pi_{\omega(q)}(\mathbf{q}) = 0 \Longrightarrow \omega(q) \sim q \quad \text{zero sound}$$

Hubbard model ($V_{\mathbf{q}} = 0$)

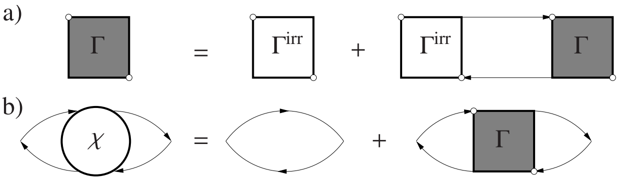
Dynamical mean-field theory: Mott transition
DOS



$m^*/m = 1/Z = 1 - \frac{d\,\mathrm{Re}\,\Sigma_\omega}{d\omega}$; $\lim_{q\to 0}\lim_{\omega\to 0}\chi_\omega(\mathbf{q}) = -dn/d\mu$



DMFT susceptibility



a)

$$\Gamma_{\nu\nu'\omega}(\mathbf{q}) = \Gamma^{\text{irr,imp}}_{\nu\nu'\omega} - T\sum_{\nu''} \Gamma^{\text{irr,imp}}_{\nu\nu''\omega}\, \chi^0_{\nu''\omega}(\mathbf{q})\Gamma_{\nu''\nu'\omega}(\mathbf{q})$$

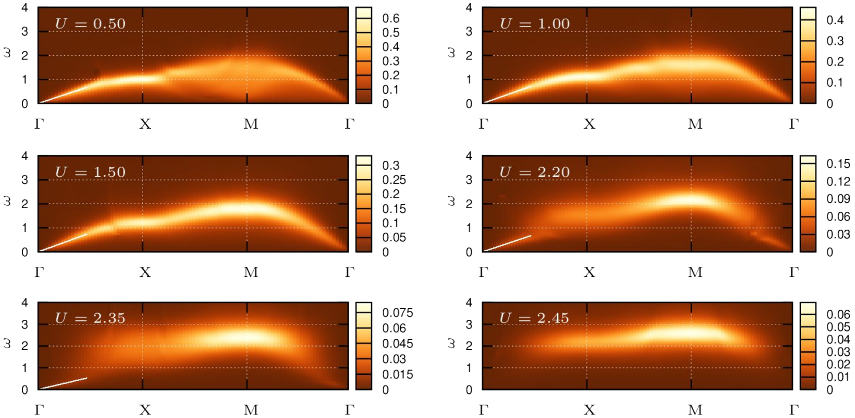
b)

$$\chi_\omega(\mathbf{q}) = 2T\sum_{\nu} \chi^0_{\nu\omega}(\mathbf{q}) - 2T^2\sum_{\nu\nu'} \chi^0_{\nu\omega}(\mathbf{q})\Gamma_{\nu\nu'\omega}(\mathbf{q})\chi^0_{\nu'\omega}(\mathbf{q})$$

[A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)]

Hubbard model ($V_{\mathbf{q}} = 0$)

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



- Zero sound mode in correlated metallic state

[HH, E. van Loon, M.I. Katsnelson, A.I. Lichtenstein and O. Parcollet, PRB **90**, 235105 (2014)]

Current

Kinetic energy: Peierls substitution

$$\hat{T} = -\tilde{t} \sum_{\mathbf{r}\boldsymbol{\delta}\sigma} c^{\dagger}_{\mathbf{r}\sigma} e^{\imath e \mathbf{A}_{\mathbf{r}} \boldsymbol{\delta}} c_{\mathbf{r}-\boldsymbol{\delta}\sigma} + c^{\dagger}_{\mathbf{r}-\boldsymbol{\delta}\sigma} e^{-\imath e \mathbf{A}_{\mathbf{r}} \boldsymbol{\delta}} c_{\mathbf{r}\sigma}$$

Invariant under gauge transformation

$$\mathbf{A}_{\mathbf{r}}\boldsymbol{\delta} \to \mathbf{A}_{\mathbf{r}}\boldsymbol{\delta} + \Lambda_{\mathbf{r}-\boldsymbol{\delta}} - \Lambda_{\mathbf{r}}, \quad c^{\dagger}_{\mathbf{r}} \to c^{\dagger}_{\mathbf{r}} e^{\imath \Lambda_{\mathbf{r}}}, \quad c_{\mathbf{r}} \to c_{\mathbf{r}} e^{-\imath \Lambda_{\mathbf{r}}}$$

Current

$$\begin{aligned}
\mathbf{j}_{\mathbf{r}} = -\frac{\delta H}{\delta \mathbf{A}_{\mathbf{r}}} =& \imath e \tilde{t} \sum_{\boldsymbol{\delta}\sigma} \left(c^{\dagger}_{\mathbf{r}\sigma} c_{\mathbf{r}-\boldsymbol{\delta}\sigma} - c^{\dagger}_{\mathbf{r}-\boldsymbol{\delta}\sigma} c_{\mathbf{r}\sigma} \right) \boldsymbol{\delta} \\
& - e^2 \tilde{t} \sum_{\boldsymbol{\delta}\sigma} \left(c^{\dagger}_{\mathbf{r}\sigma} (\mathbf{A}_{\mathbf{r}}\boldsymbol{\delta}) c_{\mathbf{r}-\boldsymbol{\delta}\sigma} + c^{\dagger}_{\mathbf{r}-\boldsymbol{\delta}\sigma} (\mathbf{A}_{\mathbf{r}}\boldsymbol{\delta}) c_{\mathbf{r}\sigma} \right) \boldsymbol{\delta} \\
=& \mathbf{j}^{\mathrm{p}}_{\mathbf{r}} + \mathbf{j}^{\mathrm{dia}}_{\mathbf{r}}
\end{aligned}$$

[R. E. Peierls, Z. Phys. **80**, 763791 (1933)]

Continuity equation

$$
\begin{aligned}
e\frac{\partial n_{\mathbf{r}}}{\partial t} =& -\imath e[n_{\mathbf{r}}, H] \\
=& \imath e\tilde{t}\sum_{\boldsymbol{\delta}\sigma}\left(c^{\dagger}_{\mathbf{r}\sigma}c_{\mathbf{r}+\boldsymbol{\delta}\sigma} + c^{\dagger}_{\mathbf{r}\sigma}c_{\mathbf{r}-\boldsymbol{\delta}\sigma} - c^{\dagger}_{\mathbf{r}+\boldsymbol{\delta}\sigma}c_{\mathbf{r}\sigma} - c^{\dagger}_{\mathbf{r}-\boldsymbol{\delta}\sigma}c_{\mathbf{r}\sigma}\right) \\
& - e^2\tilde{t}\sum_{\boldsymbol{\delta}\sigma}\left(c^{\dagger}_{\mathbf{r}\sigma}(\mathbf{A}_{\mathbf{r}}\boldsymbol{\delta})c_{\mathbf{r}+\boldsymbol{\delta}\sigma} + c^{\dagger}_{\mathbf{r}\sigma}(\mathbf{A}_{\mathbf{r}}\boldsymbol{\delta})c_{\mathbf{r}-\boldsymbol{\delta}\sigma}\right. \\
& \left. - c^{\dagger}_{\mathbf{r}+\boldsymbol{\delta}\sigma}(\mathbf{A}_{\mathbf{r}}\boldsymbol{\delta})c_{\mathbf{r}\sigma} - c^{\dagger}_{\mathbf{r}-\boldsymbol{\delta}\sigma}(\mathbf{A}_{\mathbf{r}}\boldsymbol{\delta})c_{\mathbf{r}\sigma}\right)
\end{aligned}
$$

Define *forward* derivative

$$\nabla^F \cdot \mathbf{j}_{\mathbf{r}} := \frac{\mathbf{j}_{\mathbf{r}+\boldsymbol{\delta}} - \mathbf{j}_{\mathbf{r}}}{a}$$

Continuity equation (operator identity)

$$e\frac{\partial n_{\mathbf{r}}}{\partial t} + \nabla^F \cdot \mathbf{j}_{\mathbf{r}} = 0$$

Electromagnetic response kernel $K_{\mu\nu}$

$$\langle j_\mu(q)\rangle = K_{\mu\nu}(q)A_\nu(q), \qquad j_\mu = e(n, \mathbf{j})$$

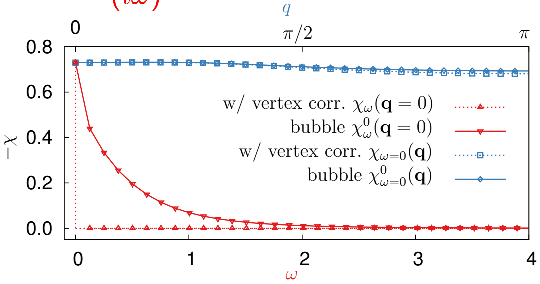
Charge conservation

$$\left\langle q^F_\mu j_\mu(q)\right\rangle = q^F_\mu K_{\mu\nu}(q)A_\nu(q) = 0 \iff q^F_\mu K_{\mu\nu}(q) = 0$$

Gauge invariance

$$K_{\mu\nu}(q)[A_\nu(q) + q^F_\nu \Lambda] = K_{\mu\nu}(q)A_\nu(q) \iff K_{\mu\nu}(q)q^F_\nu = 0$$

$$K_{00}(q) = \frac{q^2}{(\imath\omega)^2} K_{33}(q) \Longrightarrow (\imath\omega)^2\chi_\omega(\mathbf{q}=0) = 0$$



DMFT susceptibility

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)]

DMFT susceptibility

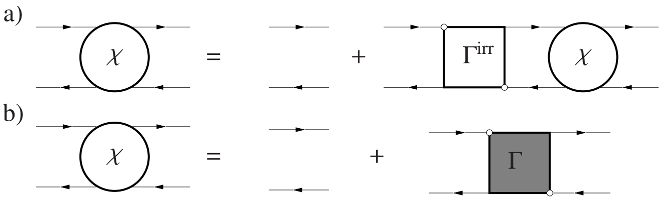
Introduce a perturbation A:

$$G^{-1} = G_0^{-1} - A - \Sigma[G]$$

Response function χ gives the *linear* change in G:

$$\chi := -\delta G/\delta A = G(\delta G^{-1}/\delta A)G$$

$$\chi = -GG - GG\frac{\delta\Sigma}{\delta A} = -GG - GG\frac{\delta\Sigma}{\delta G}\frac{\delta G}{\delta A}$$
$$= -GG + GG\Gamma^{\text{irr}}\chi$$



[G. Baym, Phys. Rev. **127**, 1391 (1962)]

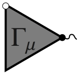
Ward identity I

Green's function analog of the continuity equation

$$\Lambda_\mu(x,y,z) = \left\langle T_\tau c(x)c^\dagger(y)j_\mu(z)\right\rangle, \quad \partial^F_\mu j_\mu = 0,$$

$$\begin{aligned}
\partial^F_\mu \Lambda_\mu =& e\left\langle T_\tau c(x)c^\dagger(y)\left[\partial_{z_0} n(z) + \nabla^F \cdot \mathbf{j}_\mathbf{r}\right]\right\rangle \\
&+ e\left\langle T_\tau c(x)[n(z), c^\dagger(y)]\delta(y_0 - z_0)\right\rangle \\
&+ e\left\langle T_\tau c^\dagger(y)[c(x), n(z)]\delta(x_0 - z_0)\right\rangle \\
=& e[\delta(x-z) - \delta(y-z)]G(x-y).
\end{aligned}$$

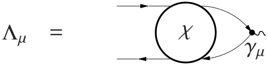
$$\Lambda_\mu(k,q) = eG(k)\Gamma_\mu(k,q)G(k+q)$$

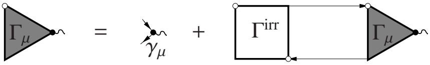


$$q^F_\mu \Gamma_\mu(k,q) = G^{-1}(k) - G^{-1}(k+q)$$

Ward identity II

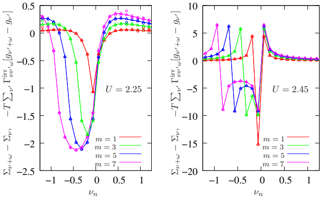
$$\Gamma_{\mu;\nu,\omega}(\mathbf{k},\mathbf{q}) = \gamma_\mu(\mathbf{k},\mathbf{q}) - T\sum_{\nu'\mathbf{k}'}\Gamma^{\text{irr}}_{\nu\nu'\omega}G_{\nu'\sigma'}(\mathbf{k}')G_{\nu'+\omega}(\mathbf{k}'+\mathbf{q})\Gamma_{\mu;\nu',\omega}(\mathbf{k}',\mathbf{q}).$$





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

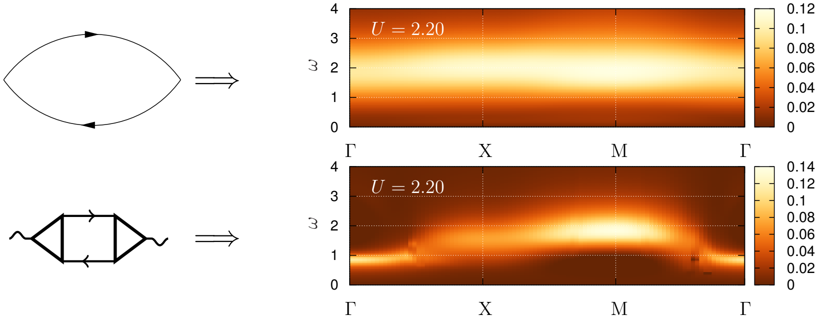
$$\times\; G_{\nu'}(\mathbf{k}')G_{\nu'+\omega}(\mathbf{k}'+\mathbf{q})[q^F_\mu\Gamma_{\mu;\nu'}(\mathbf{k}',\mathbf{q})]$$



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

$$\delta\Sigma = \frac{\delta\Sigma}{\delta g}\delta g$$

Simpler approximations



- No zero-sound mode despite short-range interaction
- Vertex corrections are crucial for long wavelength excitations
- Improper treatment of vertex corrections can lead qualitatively wrong results

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

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

$$G_\nu^{-1}(\mathbf{k}) = (g_\nu^{\text{imp}})^{-1} + \Delta_\nu - \epsilon_{\mathbf{k}}$$
$$X_\omega^{-1}(\mathbf{q}) = (\chi_\omega^{\text{imp}})^{-1} + W_\omega - V_{\mathbf{q}}$$

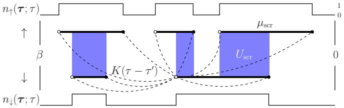
Self-consistency

$$g_\nu^{\text{imp}} = \frac{1}{N}\sum_{\mathbf{k}} G_\nu(\mathbf{k})$$
$$\chi_\omega^{\text{imp}} = \frac{1}{N}\sum_{\mathbf{q}} X_\omega(\mathbf{q})$$

[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)]

Impurity solver

Hybridization expansion CTQMC with retarded interaction U_ω and improved estimators



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

$$w_{\rm hyb}(\boldsymbol{\tau}) = \det[\Delta(\tau_i - \tau_j)]$$

$$w_{\rm at}(\boldsymbol{\tau}) = e^{-U\int_0^\beta d\tau n_\uparrow(\tau) n_\downarrow(\tau) + \mu \int_0^\beta d\tau n(\tau)} = e^{-\frac{1}{2}\sum_{ij} U_{ij} l_{ij}} e^{\mu \sum_i l_{ii}}$$

$$w_{\rm ret}(\boldsymbol{\tau}) = e^{-\int_0^\beta d\tau \int_0^\beta d\tau' n(\tau) U(\tau-\tau') n(\tau')}$$

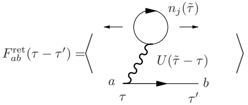
$$= e^{\frac{1}{2}\sum_{ij}\sum_{2k_{i,j}\geq\alpha_i,\alpha_j>0}^{\alpha_i\neq\alpha_j} s_{\alpha_i} s_{\alpha_j} K(\tau_{\alpha_i}-\tau_{\alpha_j})} e^{2K'(0^+)\sum_{ij}^{i\neq j} l_{ij} + K'(0^+)\sum_i l_{ii}}$$

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

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

'Bulla's trick' (inspired by use in NRG)

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

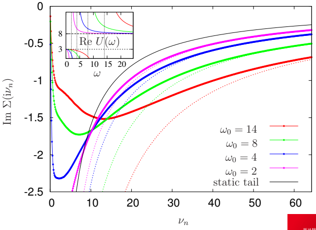


$$F_a^{\mathrm{st}}(\tau-\tau') = -\sum_j \left\langle n_j(\tau) U_{ja} c_a(\tau) c_a^*(\tau') \right\rangle$$

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

$$\sum_j \int_0^\beta d\tilde\tau\, n_j(\tilde\tau) U_{\mathrm{ret}}(\tilde\tau - \tau^e_\alpha)$$

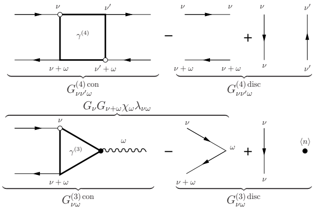
$$= -2K'(0^+) - \sum_j \sum_{\beta_j} s_{\beta_j} K'(\tau_{\beta_j} - \tau^e_\alpha)$$



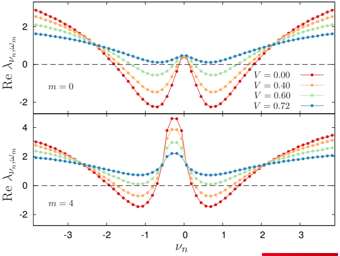
[HH, K. R. Patton, P. Werner, PRB B **85**, 205106 (2012)] [HH, Phys. Rev. B **89**, 235128 (2014)]

Improved estimator for vertex

$$G_{ab}^{(3),\mathrm{con}}(\imath\nu,\imath\omega) = \sum_i G_a(i\nu) F_{ab}^{(3)}(\imath\nu,\imath\omega) - \sum_i F'_a(\imath\nu) G_{ab}^{(3)}(\imath\nu,\imath\omega)$$



$$\lambda_a(\imath\nu,\imath\omega) = \frac{1}{\chi(\imath\omega)}\Big(\sum_b G_a^{-1}(\imath\nu) G_a^{-1}(\imath\nu+\imath\omega) \times G_{ab}^{(3),\mathrm{con}}(\imath\nu,\imath\omega) - 1\Big)$$



Model

Extended Hubbard model Hamiltonian

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

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

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

EDMFT:

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

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

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

vs. RPA:

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

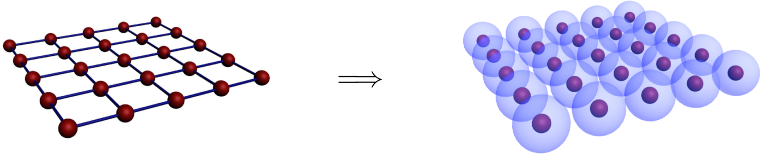
$$1 + V\Pi_{\omega(q)}(\mathbf{q})/q^2 = 0$$

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

Dual bosons: basic idea

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

Introduce impurity problem at each lattice site



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

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

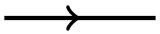
[A.N. Rubtsov, M.I. Katsnelson, A.I. Lichtenstein, Ann. Phys. **327**, 1320 (2012)]

Dual perturbation theory

$$\tilde{S}[f^*,f;\phi] = -\sum_{\mathbf{k}\nu\sigma} f^*_{\mathbf{k}\nu\sigma}\tilde{\mathcal{G}}^{-1}_{\mathbf{k}\nu\sigma} f_{\mathbf{k}\nu\sigma} - \frac{1}{2}\sum \phi_{\mathbf{q}\omega}\tilde{\mathcal{X}}_{\mathbf{q}\omega}\phi_{\mathbf{q}\omega} + \sum_i \tilde{V}^i[f^*,f;\phi]$$

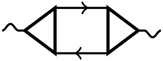
$$\tilde{V}^i[f^*,f;\phi] = \sum_{\nu\omega\sigma} \lambda^{\sigma}_{\nu\omega} f^*_{\nu\sigma} f_{\nu+\omega\sigma}\phi_\omega - \frac{1}{4}\sum_{\nu\nu'\omega\sigma_j} \gamma^{\sigma_1\sigma_2\sigma_3\sigma_4}_{\nu\nu'\omega} f^*_{\nu\sigma_1} f_{\nu+\omega\sigma_2} f^*_{\nu'+\omega\sigma_3} f_{\nu'\sigma_4}$$

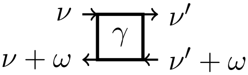
Evaluate fermionic and bosonic self-energies $\tilde{\Sigma}$, $\tilde{\Pi}$
in dual perturbation theory



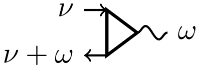
(b) $\tilde{G}^{(0)}_{\mathbf{k}\nu}$

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





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



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

Polarization corrections

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

$$G^{-1}_{\mathbf{k}\nu} = g^{-1}_{\nu}(1 + \tilde{\Sigma}_{\mathbf{k}\nu} g_{\nu})^{-1} + \Delta_{\nu} - \epsilon_{\mathbf{k}}$$
$$X^{-1}_{\mathbf{q}\omega} = \chi^{-1}_{\omega}(1 + \tilde{\Pi}_{\mathbf{q}\omega} \chi_{\omega})^{-1} + W_{\omega} - V_{\mathbf{q}}$$

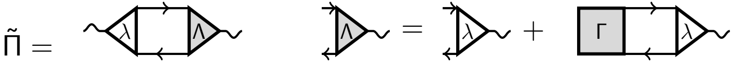
Define physical polarization:

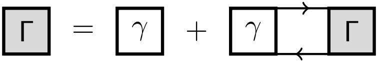
$$X^{-1}_{\mathbf{q}\omega} = -\Pi^{-1}_{\mathbf{q}\omega} - V_{\mathbf{q}}$$

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

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

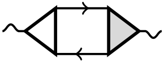
This talk: $\tilde{\Sigma} = 0$,

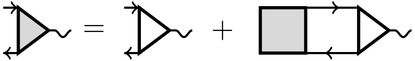


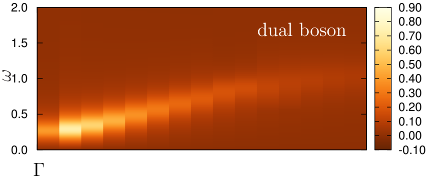


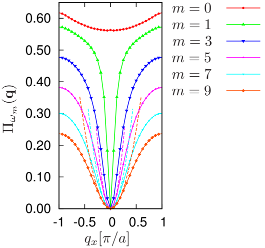
Exactly equivalent to DMFT susceptibility for $V = 0$

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

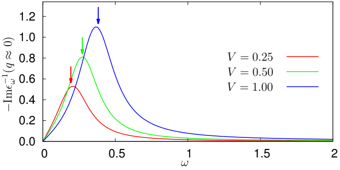








Dual boson polarization
$\Pi_\omega(\mathbf{q}) \sim q^2 \ (\omega > 0)$



Plasma frequency:

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

Model

Extended Hubbard model Hamiltonian

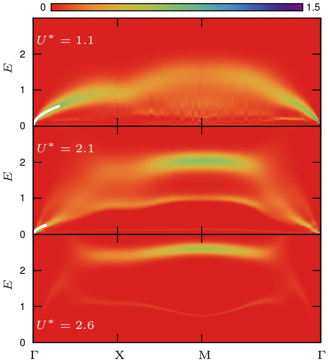
$$H = -\tilde{t} \sum_{\mathbf{r}\delta\sigma} \left(c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}-\delta\sigma} + c^\dagger_{\mathbf{r}-\delta\sigma} c_{\mathbf{r}\sigma} \right) + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} + \frac{1}{2} \sum_{\mathbf{r}\mathbf{r}'} V(\mathbf{r}-\mathbf{r}')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

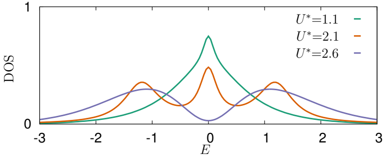
$\mathbf{r}$: <u>discrete</u> lattice site positions; half bandwidth $D = 1$

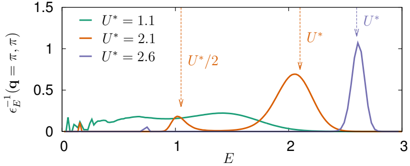
- $V_{\mathbf{q}} = 0$ local interaction $\rightarrow$ Hubbard model (2D)
- $V_{\mathbf{q}} = \frac{V}{q^2}$, (screened) Coulomb interaction (3D)
- $V_{\mathbf{q}} = \frac{V}{q}$, (screened) Coulomb interaction (2D)
- $V_{\mathbf{q}} = 2V(\cos q_x + \cos q_y)$, nearest-neighbor interaction (2D)

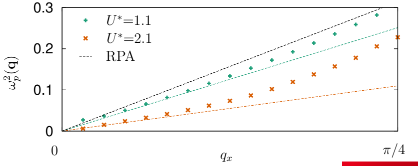
Surface plasmons: $(V_{\mathbf{q}} = V/q)$

Spectral weight transfer and renormalized dispersion









Plasma frequency does *not* scale with quasiparticle weight Z

[E. van Loon, HH, A. I. Lichtenstein, A. N. Rubtsov, M. I. Katsnelson, PRL **113**, 246407 (2014)]

Model

Extended Hubbard model Hamiltonian

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

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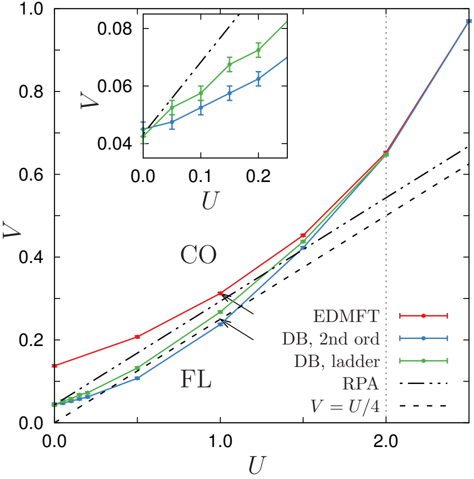
- $V_{\mathbf{q}} = \frac{V}{q}$, (screened) Coulomb interaction (2D)
- $V_{\mathbf{q}} = 2V(\cos q_x + \cos q_y)$, nearest-neighbor interaction (2D)

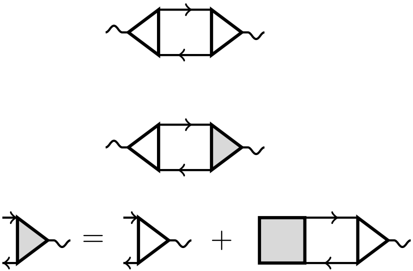
Extended Hubbard model: $U - V$ phase diagram (2D)

Transition to charge-ordered (CO) insulator



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

Dual boson diagrams:

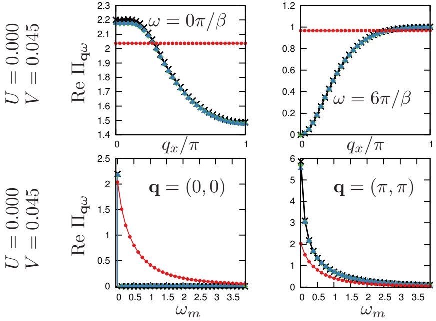


- Large corrections to EDMFT even for small U
- RPA is reproduced non-trivially for $U \to 0$!

[E. van Loon, A. I. Lichtenstein, M. I. Katsnelson, O. Parcollet, HH, PRB **90**, 235135 (2014)]

Polarization

U=0



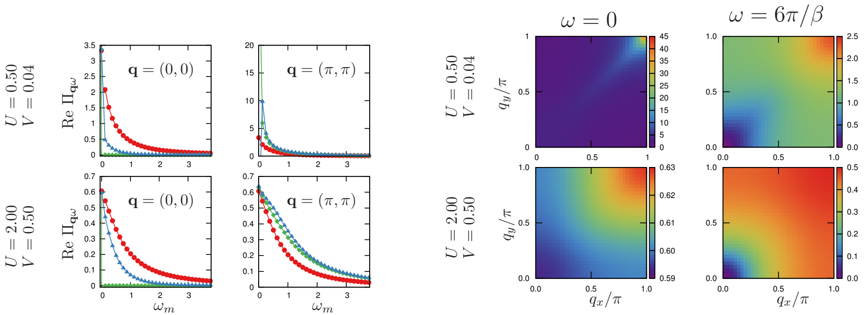
RPA

$$X_{\mathbf{q}\omega} = \frac{1}{-\Pi^{-1}_{\mathbf{q}\omega} - (U + V_{\mathbf{q}})}.$$

$$\Pi^{\text{RPA}}_{\mathbf{q}\omega} = -\frac{T}{N}\sum_{\mathbf{k}\nu\sigma} G^{(0)}_{\mathbf{k}\nu} G^{(0)}_{\mathbf{k}+\mathbf{q}\nu+\omega}$$

- At weak coupling, dual boson (blue) essentially reproduces RPA (black)
- EDMFT (red) polarization deviates significantly

Polarization



(ladder approximation)

- Charge conservation violated in EDMFT (red) and second-order DB (blue); more severe at large U
- Artifacts in second-order DB
- EDMFT and DB are close at strong coupling

Simplified dual boson (s-DB)

Neglect two-particle vertex: $\gamma = 0$

$$\lambda^{\sigma}_{\nu\omega} = \frac{1}{\chi_\omega}\left(T\sum_{\nu'\sigma'}\gamma^{\sigma\sigma'}_{\nu\nu'\omega} g_{\nu'\sigma'} g_{\nu'+\omega,\sigma'} - 1\right)$$

$$\lambda^{\sigma}_{\nu\omega} \to -\chi^{-1}_\omega$$

This yields an approximation similar to EDMFT+GW (V=decoupling):

s-DB

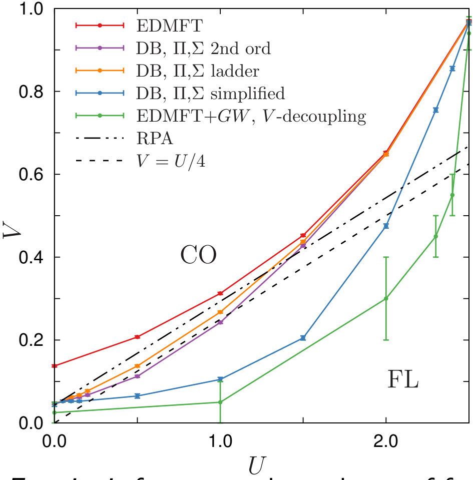
$$\Pi^{-1}_{\mathbf{q}\omega} = -(\chi_\omega + \{GG\}^{\text{nonloc}}_{\mathbf{q}\omega})^{-1} - W_\omega.$$

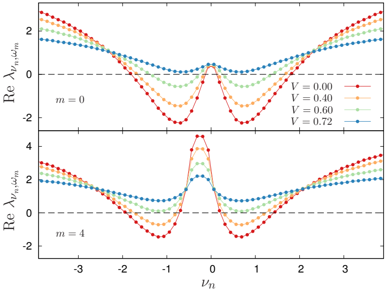
EDMFT+GW

$$\Pi^{-1}_{\mathbf{q}\omega} = \left[\left(-\chi^{-1}_\omega - W_\omega\right)^{-1} - \{GG\}^{\text{nonloc}}_{\mathbf{q}\omega}\right]^{-1}$$

$U - V$ phase diagram

Transition to charge-ordered (CO) insulator: $X^{-1}_{\mathbf{q}=(\pi,\pi),\omega=0} = 0$





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

Fermionic frequency-dependence of fermion-boson vertex is important!

Conclusions

- DMFT susceptibility appears to be conserving in finite dimensions, EDMFT is not
- Neglect of vertex corrections can lead to qualitatively wrong results
- Frequency dependent self-energy requires frequency dependent irreducible vertex
- Dual boson approach includes vertex corrections beyond RPA and describes zero sound / plasmons in correlated state
- Three-leg vertex is important

References:

- Collective excitations and gauge invariance: H. Hafermann, E. van Loon, M. I. Katsnelson, A. I. Lichtenstein and O. Parcollet, Phys. Rev. B **90**, 235105 (2014).
- Spectral weight transfer and renormalized dispersion: E. van Loon, H. Hafermann, A. I. Lichtenstein, A. N. Rubtsov, M. I. Katsnelson, Phys. Rev. Lett. **113**, 246407 (2014).
- Dual boson application to extended Hubbard model: E. van Loon, A. I. Lichtenstein, M. I. Katsnelson, O. Parcollet, H. Hafermann, Phys. Rev. B **90**, 235135 (2014).

Thank you for your attention !