Dual fermions: a nonlocal extension to DMFT with a high momentum resolution

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in cooperation with

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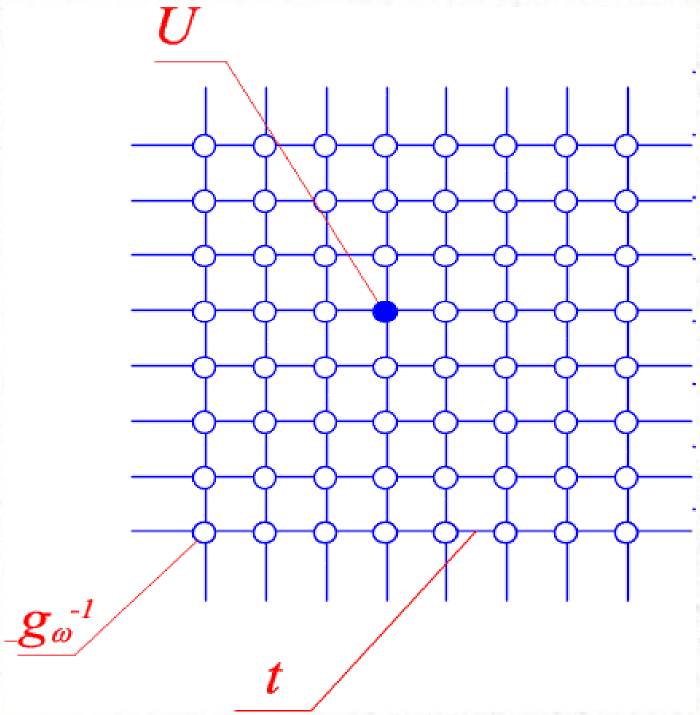
Local nature of DMFT



$$g_\omega = \sum_k \frac{N^{-1}}{g_\omega^{-1} - \epsilon_k + \Delta_\omega}$$

$$G_{\omega k} = \frac{1}{g_\omega^{-1} - \epsilon_k + \Delta_\omega}$$

DMFT self-energy is local

Impurity problem

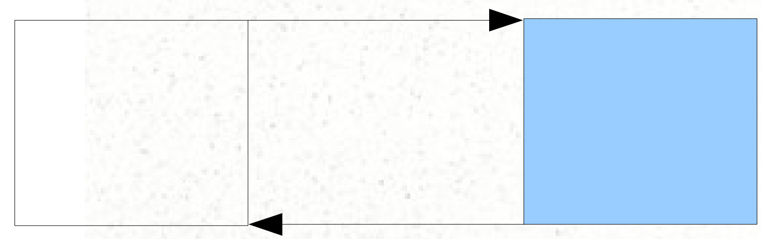
$$S_{imp} = \sum_{\omega,\sigma} (\Delta_\omega - \mu - i\omega) c^*_{\omega,\sigma} c_{\omega,\sigma} + U \int_0^\beta n_{\uparrow\tau} n_{\downarrow\tau} d\tau$$

is described by Green's function $g_{\tau-\tau'} = - < T c_\tau c^*_{\tau'} >$ only

Something nonlocal of DMFT...

A transition condition: instability with respect to variations of Δ

$$\delta g_\omega = \sum \delta \left(\frac{N^{-1}}{g_\omega^{-1} + \Delta_\omega - \epsilon_k} \right)$$



$$\delta g_\omega = \chi_{\omega\omega'} \delta_{\Delta} \omega'$$

$$\det \left(N^{-1} \sum_k (G_{\omega k} - g_\omega)^2 \gamma^{(4)}_{\omega\omega'} - 1 \right) = 0$$

Transition points and susceptibilties in DMFT are related with ladder sums

On the route to construct a nonlocal extension of DMFT

Since DMFT uses only the Green's function
of the impurity problem,
its reasonable to construct an expansion in higher
vertex parts:
zeroth order of such series would coincide with DMFT

Other ways to describe nonlocality

- •Cluster methods
- •Integral ladder-like equations
- •Introduce classical fluctuations to describe AF modes

Our method is a simple way to describe
short- and long- range nonlocality at equal footing;
It provides a regular way to construct high approximations

Mathematics

Start with partition function $Z = \int e^{-S[c,c^*]}\mathcal{D}c^*\mathcal{D}c$ubbard action

$$S[c,c^*] = -\sum_{i\omega,\sigma}(\mu + i\omega)c^*_{i,\omega,\sigma}c_{i,\omega,\sigma} + U\int_0^\beta n_{i,\uparrow,\tau}n_{i,\downarrow,\tau}d\tau + \sum_{\omega k\sigma}\epsilon_k c^*_{\omega k\sigma}c_{\omega k\sigma}$$

Rewrite it

$$S[c,c^*] = \sum_i S_{imp}[c_i,c_i^*] - \sum_{\omega k\sigma}(\Delta_\omega - \epsilon_k)c^*_{\omega k\sigma}c_{\omega k\sigma}$$

$$S_{imp}[c_i,c_i^*] = \sum_{\omega,\sigma}(\Delta_\omega - \mu - i\omega)c^*_{i,\omega,\sigma}c_{i,\omega,\sigma} + U\int_0^\beta n_{i,\uparrow,\tau}n_{i,\downarrow,\tau}d\tau$$

Decouple the Gaussian part, using the identity

$$e^{A^2 c^*_{\omega k\sigma}c_{\omega k\sigma}} = B^{-2}\int e^{-AB(c^*_{\omega k\sigma}f_{\omega k\sigma} + f^*_{\omega k\sigma}c_{\omega k\sigma}) - B^2 f^*_{\omega k\sigma}f_{\omega k\sigma}}df^*_{\omega k\sigma}df_{\omega k\sigma}$$

It gives an action

$$S[c,c^*,f,f^*] = \sum_i S_{imp}[c_i,c_i^*] +$$

$$\sum_{\omega k\sigma}\left[g_\omega^{-1}(f^*_{\omega k\sigma}c_{\omega k\sigma} + c^*_{\omega k\sigma}f_{\omega k\sigma}) + g_\omega^{-2}(\Delta_\omega - \epsilon_k)^{-1}f^*_{\omega k\sigma}f_{\omega k\sigma}\right]$$

<u>That allows to integrate over *c*, *c** at each site separately</u>

This integration gives

$$S[f,f^*] = \sum_{\omega k\sigma} g_\omega^{-2} \left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega \right) f^*_{\omega k\sigma} f_{\omega k\sigma} + \sum_i V_i$$

$$e^{-V[f_j,f_j^*] - g_\omega^{-1} f^*_{j\omega} f_{j\omega}} = \int e^{-S_{imp}[c_j,c_j^*] + g_\omega^{-1}(f^*_{\omega k\sigma} c_{\omega k\sigma} + c^*_{\omega k\sigma} f_{\omega k\sigma})} \mathcal{D}c_j^* \mathcal{D}c_j$$

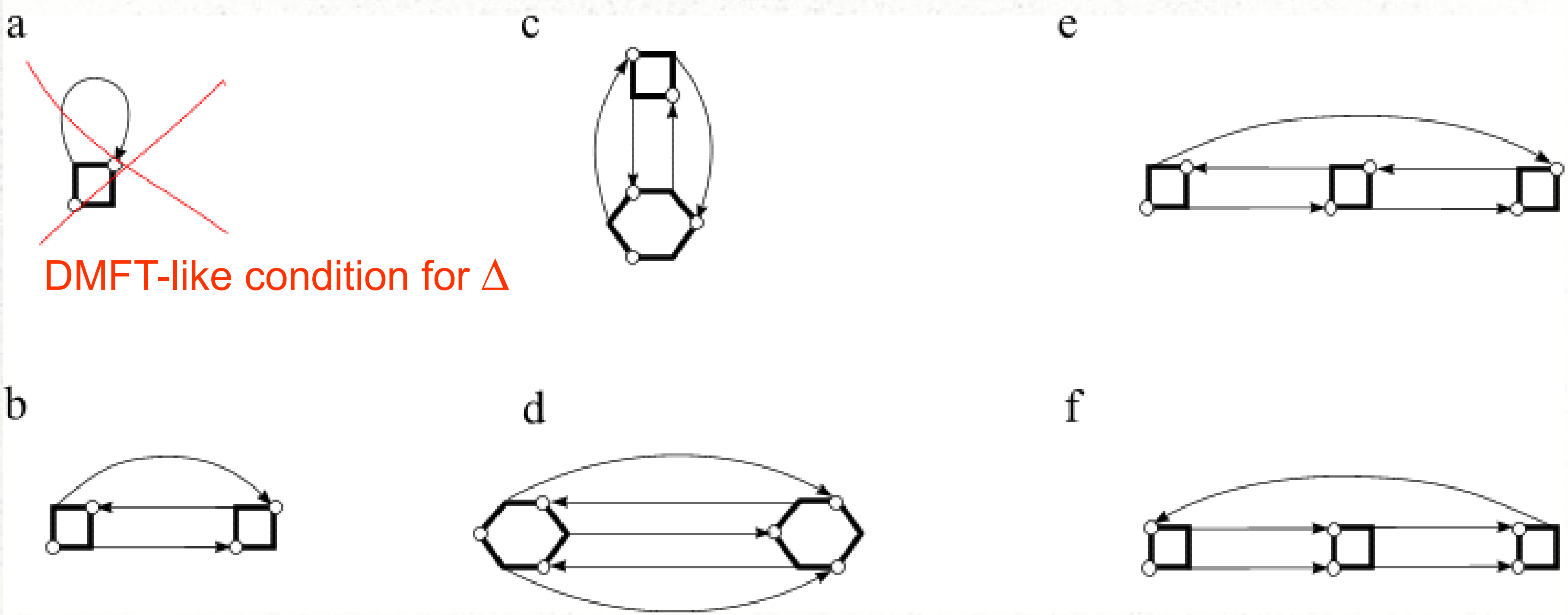
$$V[f_i,f_i^*] = -\gamma^{(4)}_{1234} f_1^* f_2 f_3^* f_4 + \gamma^{(6)}_{123456} f_1^* f_2 f_3^* f_4 f_5^* f_6 + \ldots$$

In principle, these expressions solve the problem:
In the new variables, an expansion in the nonlinear part of action is actually an expansion with respect to irreducible vertices of a impurity problem.

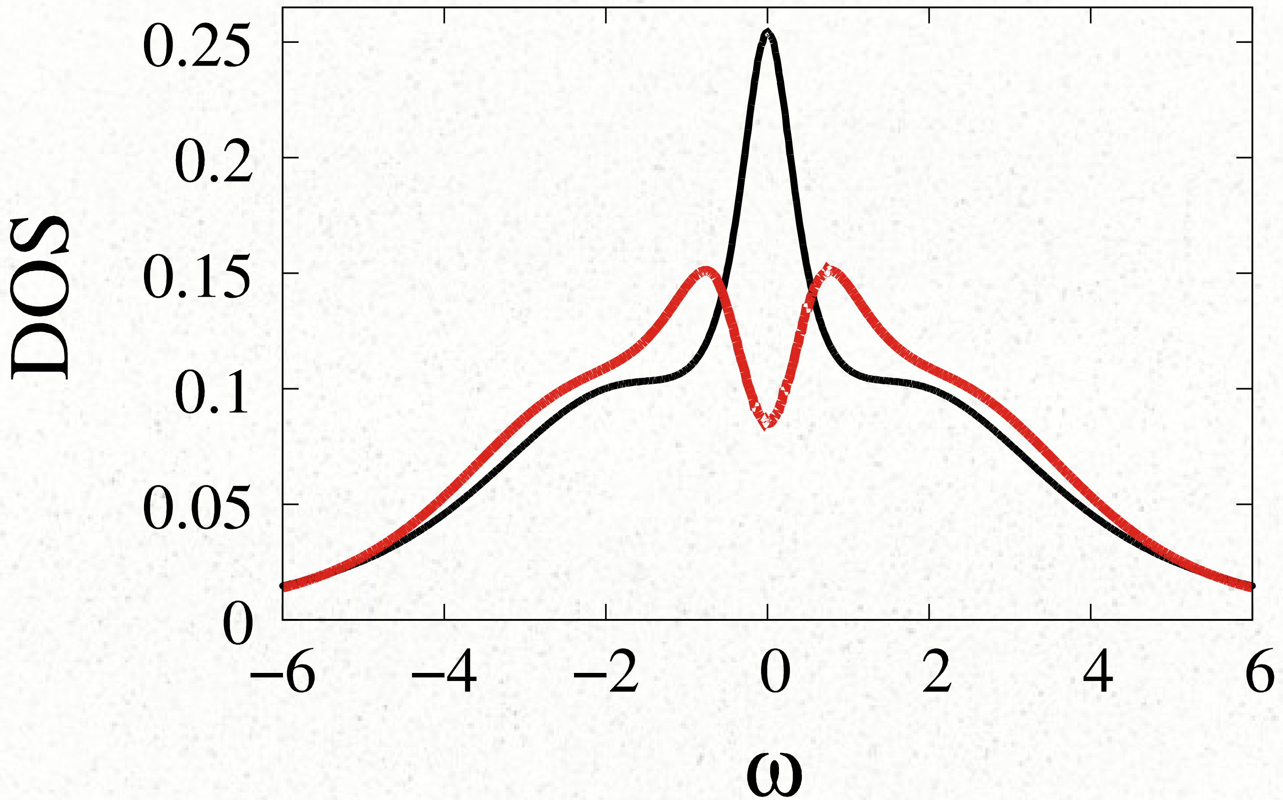
Once the problem is solved in new variables, its easy to return to the initial ones: there is an exact relation between lattice Green's functions

$$G_{\omega,k} = g_\omega^{-2} (\Delta_\omega - \epsilon_k)^{-2} G^{dual}_{\omega,k} + (\Delta_\omega - \epsilon_k)^{-1}$$

Low-order diagrams for the dual self energy



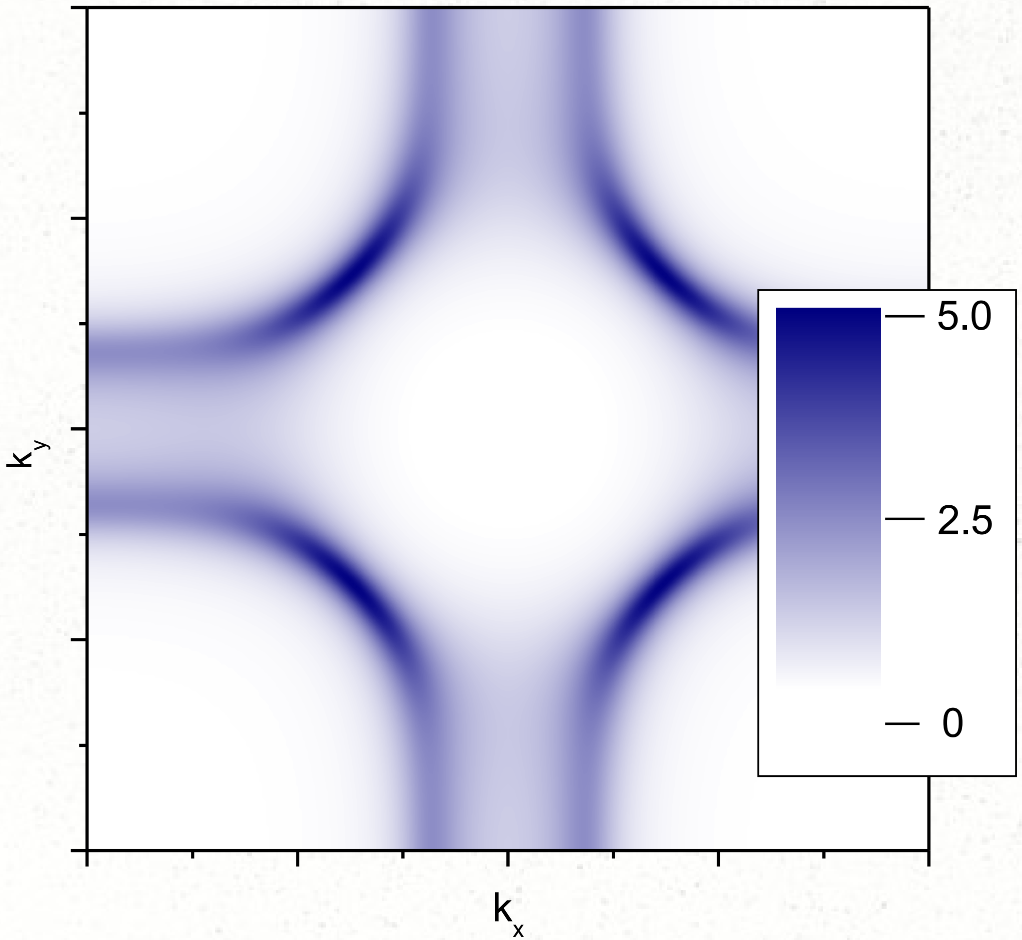
Antiferromagnetic pseudogap



DMFT (black line), and dual-fermion AF ladder (red line) DOS at $U/t=4$, $\beta t=5$. The dual-fermion DOS exhibits an antiferromagnetic pseudogap.

H. Hafermann, G. Li, A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, and H. Monien
Phys. Rev. Lett. 102, 206401 (2009)

Spectral density at Fermi level for doped t-t' Hubbard model

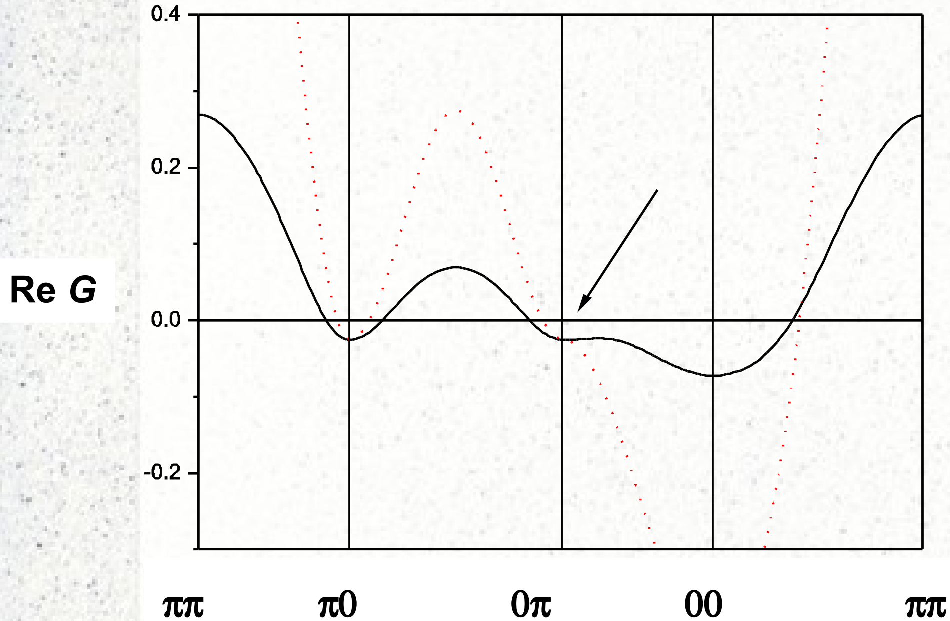


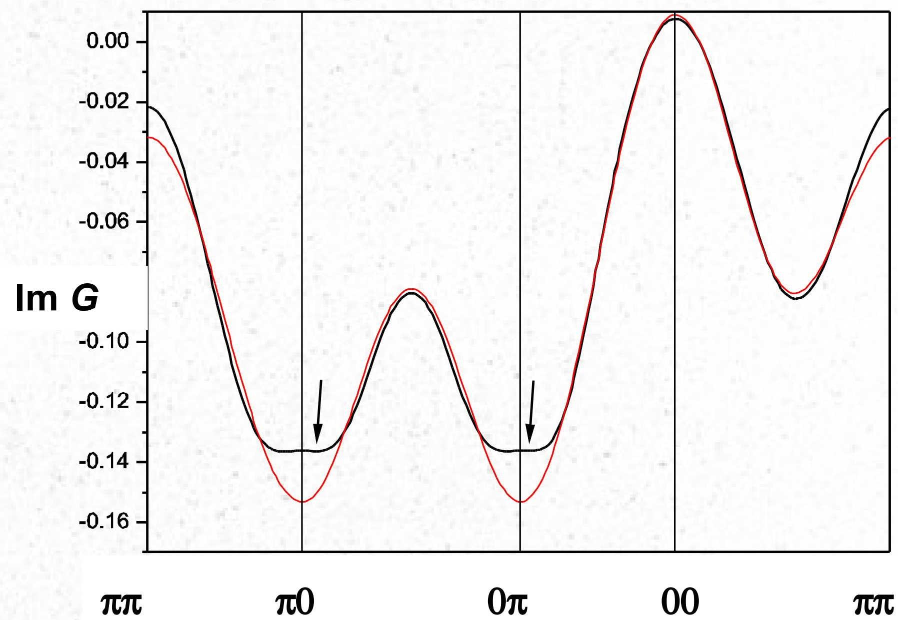
U=4.0, t=0.25, t'=-0.075
β=80
14% doping

Calculations with diagram (b)

A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, and A. Georges
Phys. Rev. B 79, 045133 (2009)

Renormalization of the spectral function near Van Hove singuliarities





U=4.0, t=0.25, t'=-0.075
β=80
14% doping

To summarize

Low-order dual diagrams are responsible for nonlocal self-energy renormalization, in particular in the the narrow regions of Fermi surface (van Hove physics).

Ladder diagrams are important to describe the electron dispersion near the phase transition (listen to H. Hafermann's talk).

Simple ladder summation should NOT improve the DMFT phase diagram drastically, because its contribution to the susceptibility is already taken into account in the DMFT self-consistency condition. More saphisticated diagram series are required to describe the phase diagram beyond DMFT.