Dual-fermion approach to spatial nonlocality of correlated electrons

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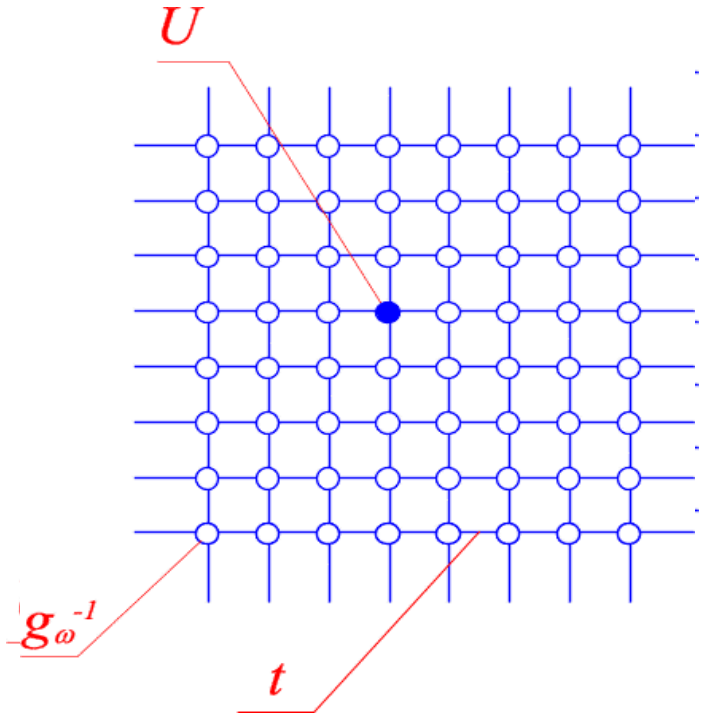
Methodologically, the talk will be about
a perturbation expansion on top of the dynamical mean-field theory

DMFT

An analog of the coherent-potential approach for disordered media

W. Metzner, D. Vollhardt (1989) G. Kotliar, A. Georges (1993)

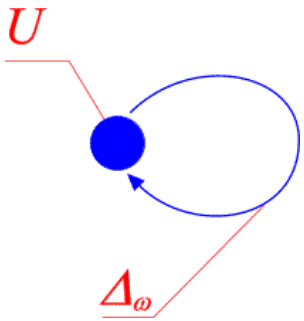


$$g_\omega = \sum_k \frac{N^{-1}}{g_\omega^{-1} - \epsilon_k + \Delta_\omega}$$

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

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 $g_{\tau-\tau'} = -<Tc_\tau c^*_{\tau'}>$ only

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

Mathematics

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

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

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

That allows to integrate over *c*, *c** at each site separately

Series for $V(c^*,c)$

This integration gives

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

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

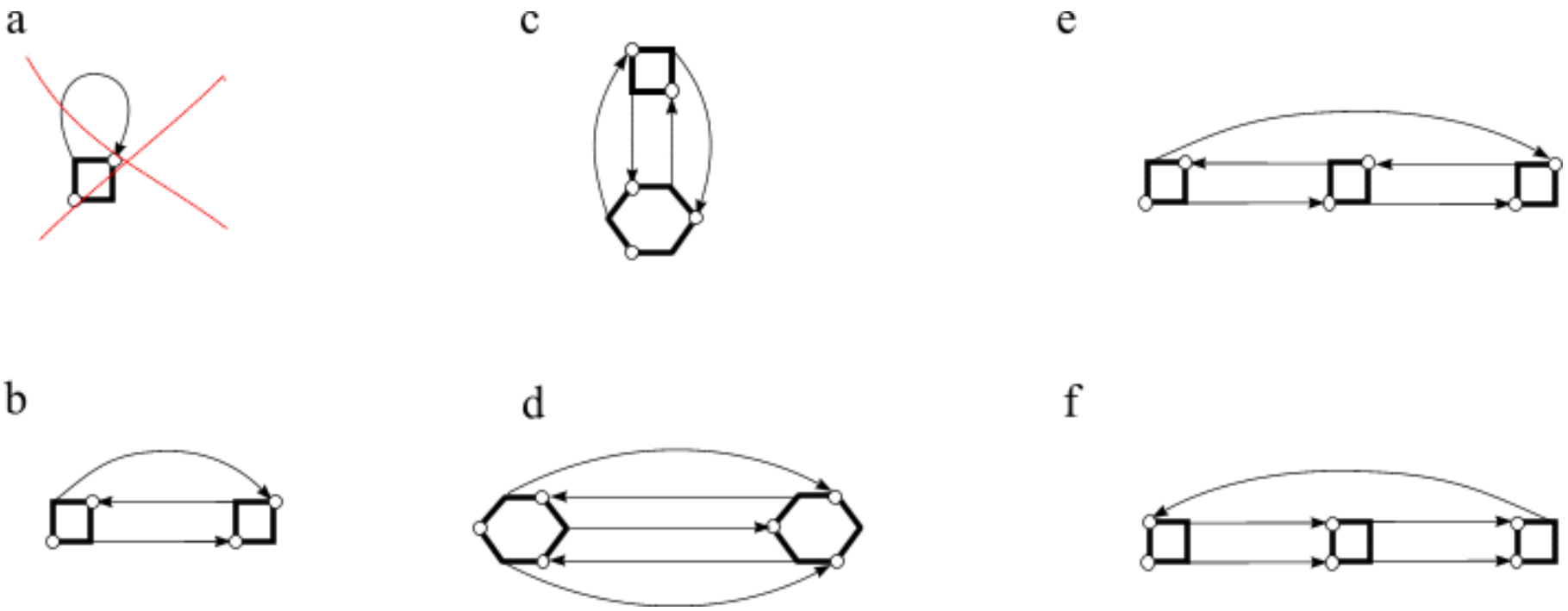
$$V[f_i,f_i^*] = -\gamma^{(4)}_{1234}f_1^*f_2f_3^*f_4 + \gamma^{(6)}_{123456}f_1^*f_2f_3^*f_4f_5^*f_6 + \ldots$$

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



Limiting cases

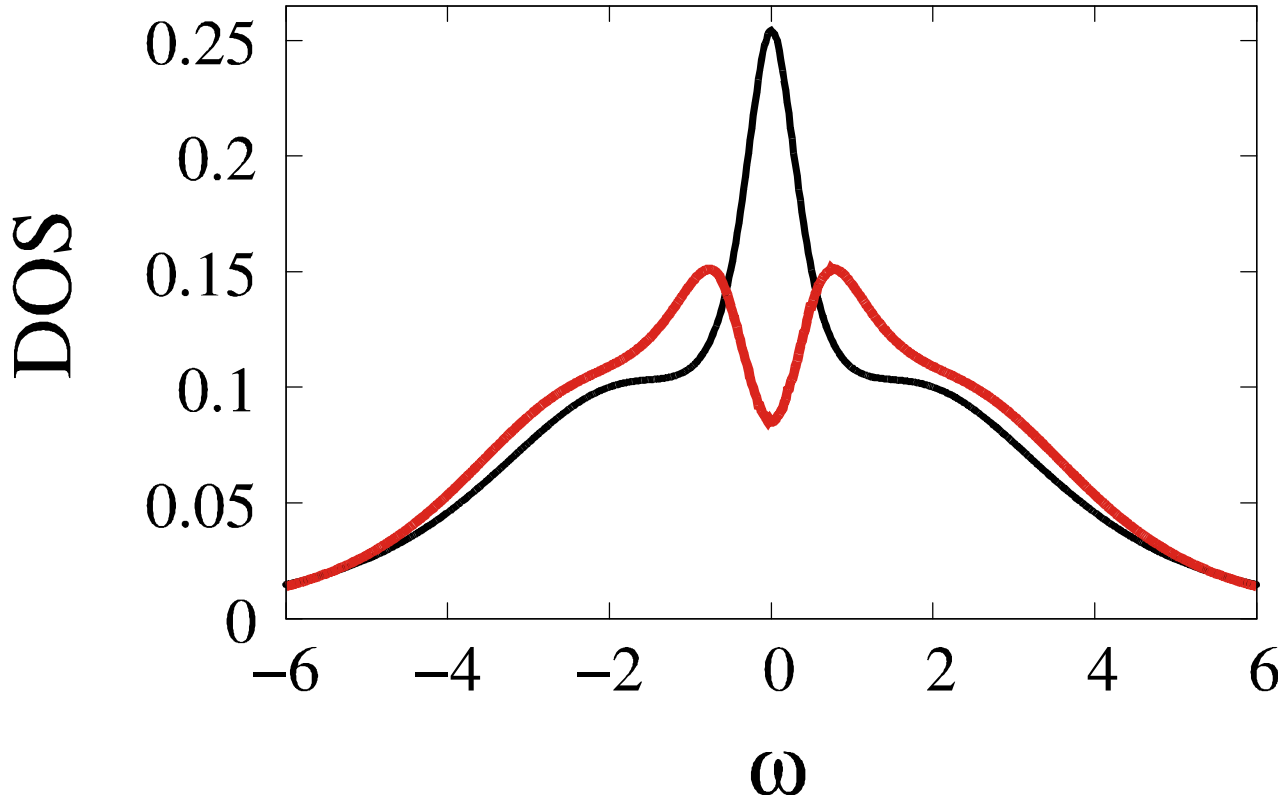
Vertexes of diagrams are small for weak-coupling limit

There is no spatial dispersion in atomic limit, so $\sum_k G_{dual} = 0$ means vanishing of the evtire G_{dual}

Near atomic limit, lines in diagrams are small

There is a good interpolation between the two limits

Antiferromagnetic pseudogap



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

Modeling the Fermi arc in underdoped cuprates

M. R. Norman,[1] A. Kanigel,[2] M. Randeria,[3] U. Chatterjee,[2] and J. C. Campuzano[2,1]

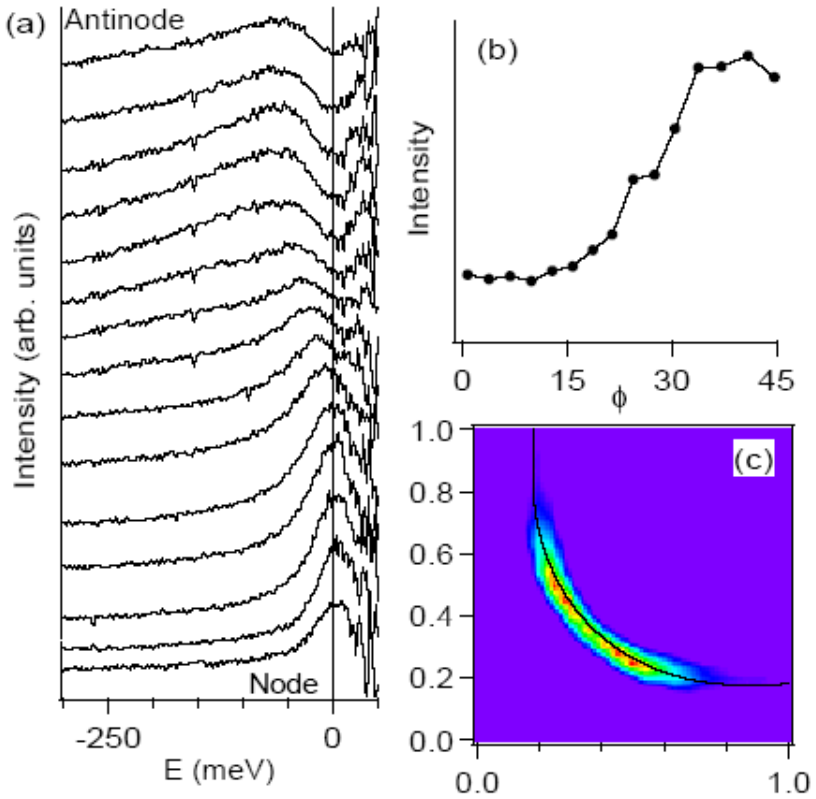
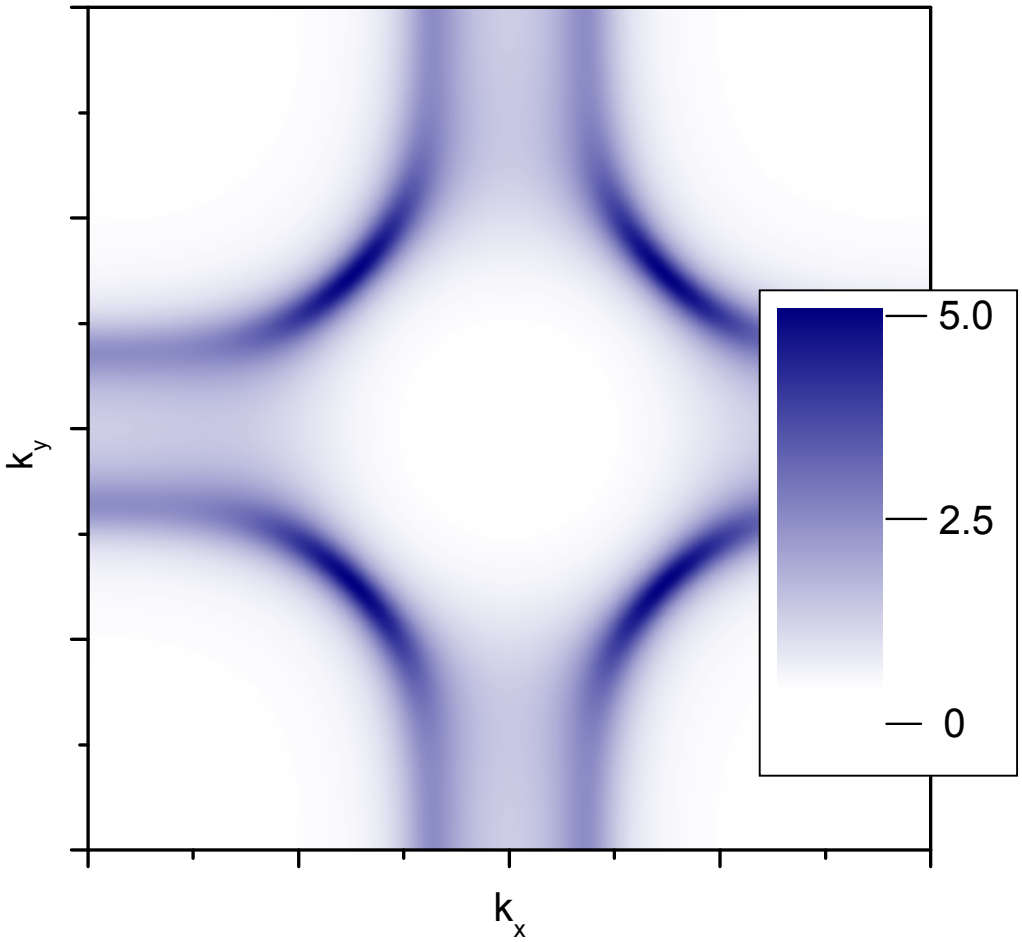


FIG. 2: (Color online) (a) Experimental energy distribution curves (EDCs) for optimal doped $Bi_2Sr_2CaCu_2O_8$ (Bi2212) around the underlying Fermi surface in the pseudogap phase (T=140K) divided by a resolution broadened Fermi function.

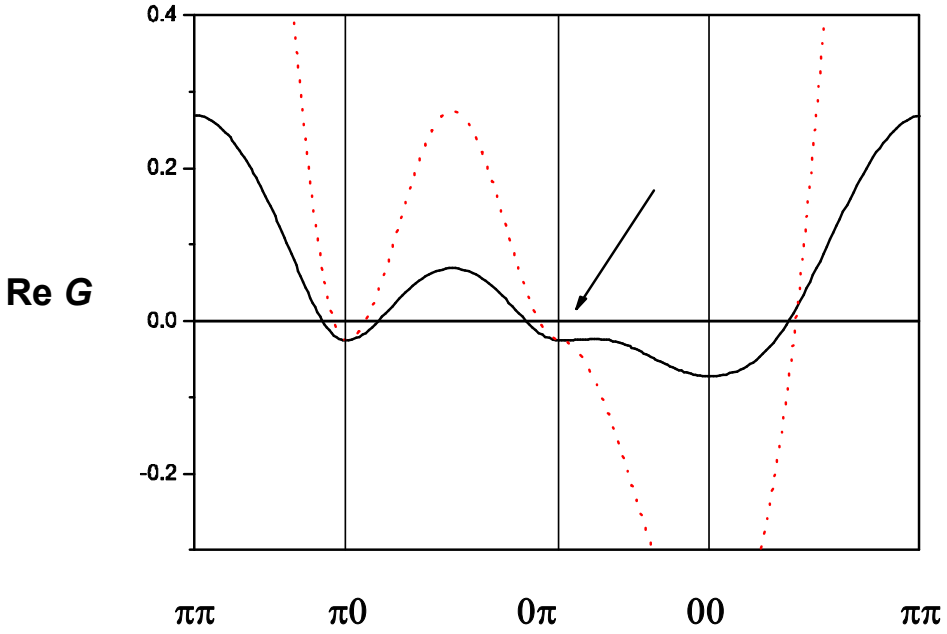
Spectral density at Fermi level for doped t-t' Hubbard model

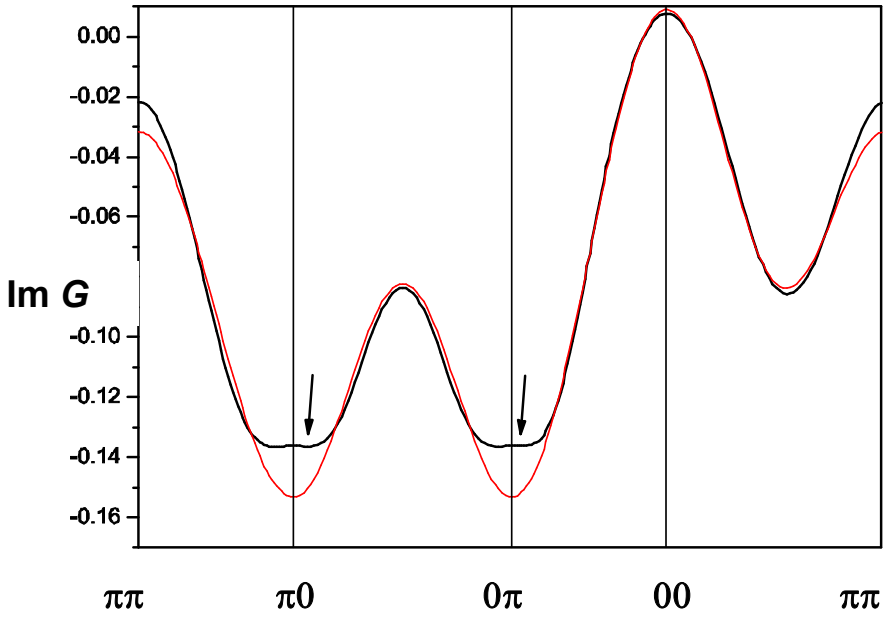


U=4.0, t=0.25, t'=-0.075
β=80
14% doping

Calculations with diagram (b)

Renormalization of the spectral function near Van Hove singuliarities



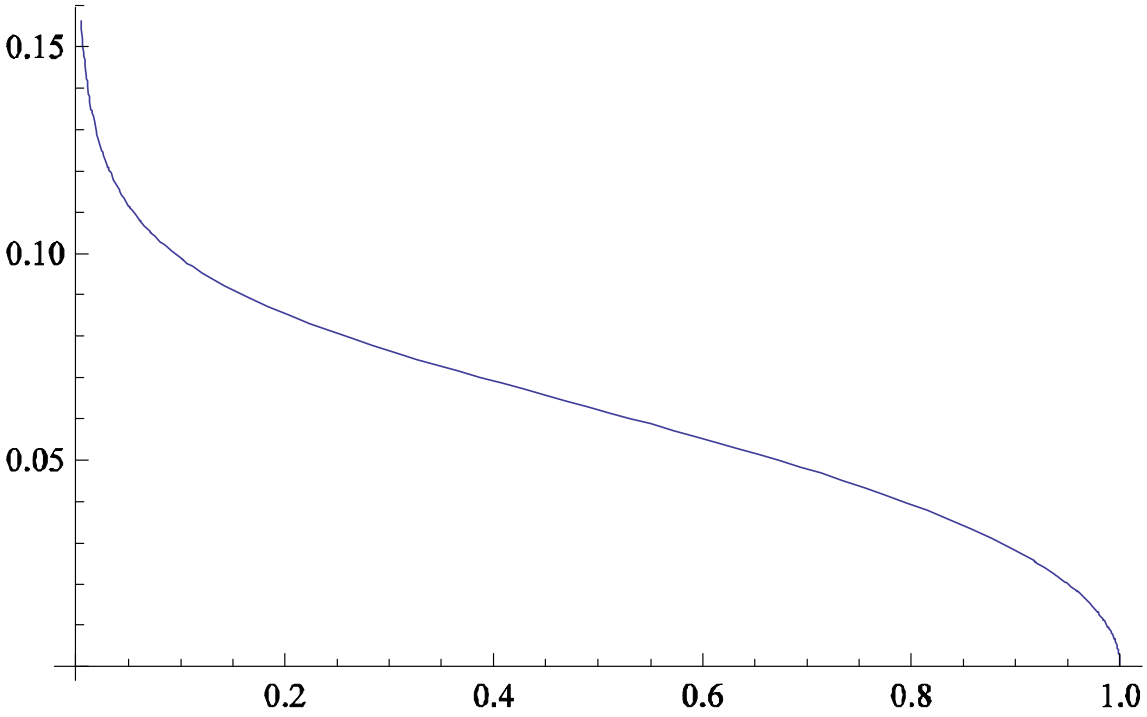


U=4.0, t=0.25, t'=-0.075
β=80
14% doping

Decoupling of the hybridization in the impurity problem

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

Certain change of formalism, because atomic problem is Hamiltonian, with a degenerate ground state.



- 1st order correction:
- Kondo logarithm
- Friedel sum rule

Thanks