A new approach for strongly correlated fermions combining FRG with DMFT

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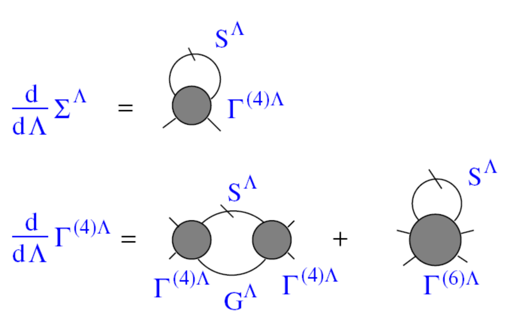
FRG APPROACH

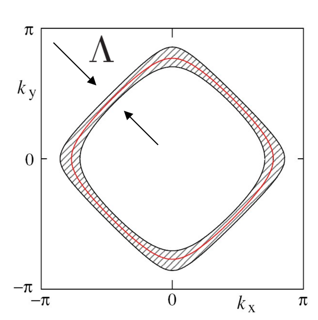
- The functional renormalization group (fRG) is based on an exact field theoretic equation for a generating functional [1]

$$\frac{d}{d\Lambda}\Gamma^\Lambda[\psi,\overline{\psi}] = -\left(\overline{\psi},\dot{Q}_0^\Lambda\psi\right) - \mathrm{tr}\left(\dot{Q}_0^\Lambda\left[\frac{\delta^2\Gamma^\Lambda}{\delta\overline{\psi}\delta\psi}\right]^{-1}\right)$$

- Inverse propagator, which includes cutoff $Q_0^\Lambda(k_0,\mathbf{k}) = [G_0^\Lambda(k_0,\mathbf{k})]^{-1}$
- Hierarchy of differential equations for vertex functions (truncation is necessary)



- Unbiased analysis of competing instabilities is possible

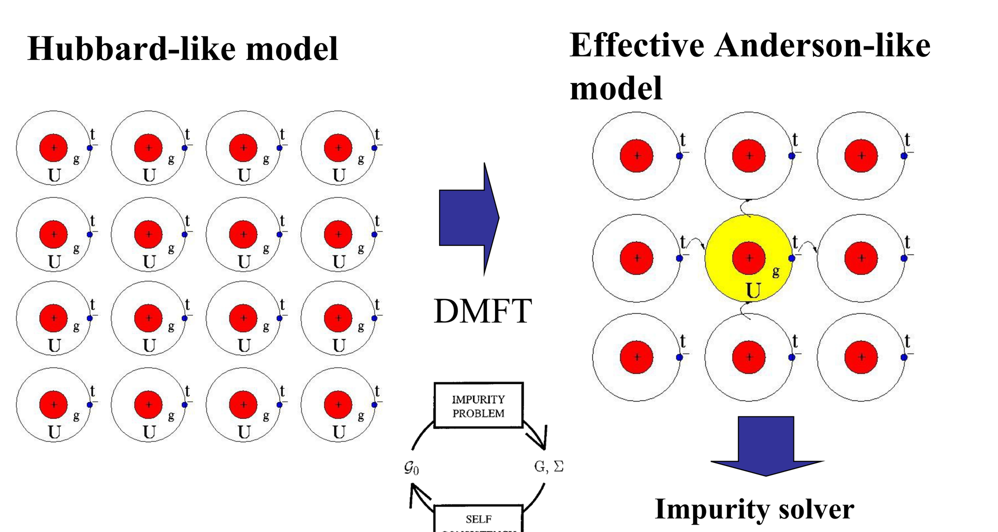


- Successfully applied in many situations [1] (2d Hubbard model, pnictides, graphene)

Disadvantage: Application of fRG is usually restricted to weak coupling

DMFT APPROACH

- Lattice model is described by effective impurity model and self-consistency condition



- Effective action [2]

$$S_{\rm eff} = -\int_0^\beta d\tau\int_0^\beta d\tau'\sum_\sigma c^\dagger_{0,\sigma}(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_{0,\sigma}(\tau') + U\int_0^\beta d\tau\, n_{0,\uparrow}(\tau)n_{0,\downarrow}(\tau)$$

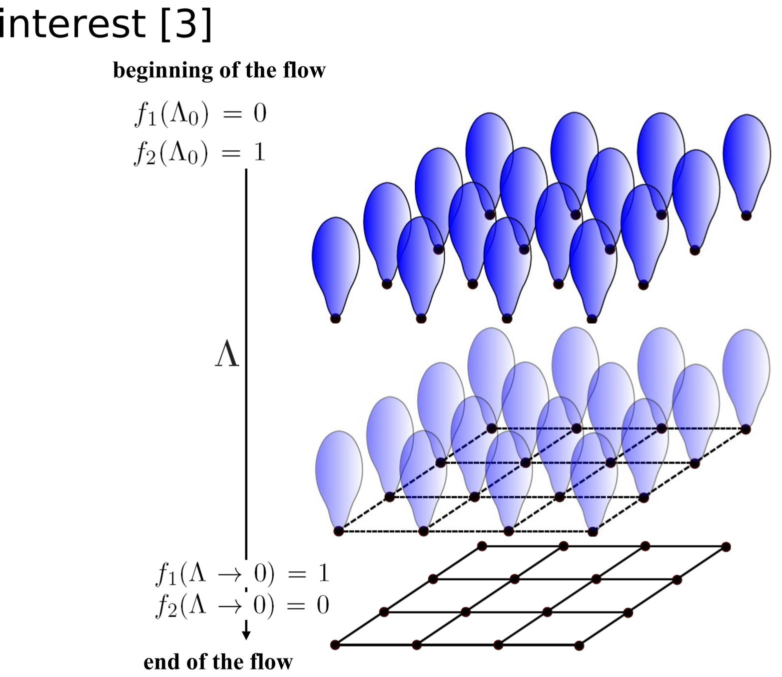
$$\tilde{\mathcal{G}}_0^{-1}(z) = z - \varepsilon_d - K(z)$$ Describes bath

- Exact in the limit of infinite dimensions
- Non-perturbative solutions can access strong coupling regime (e.g. Mott physics)

Disadvantage: Non-local correlations are neglected entirely

COMBINING FRG AND DMFT

- FRG scheme is very abstract, so any flow in the quadratic part can be implement
- Idea: Flow from DMFT limit to (2d) model of interest [3]



$$S_{2d}^\Lambda[c_{i,\sigma}(t),\overline{c}_{i,\sigma}(t)] = \int_0^\beta d\tau\sum_{i,j,\sigma}\overline{c}_{i,\sigma}(\tau)\Big(\delta_{ij}\frac{\partial}{\partial\tau} - t_{ij}f_{1,ij}(\Lambda) - \delta_{ij}\mu - K(\tau)\delta_{ij}f_2(\Lambda)\Big)c_{j,\sigma}(\tau) + U\sum_i n_{i\uparrow}(\tau)n_{i\downarrow}(\tau)$$

- Inverse propagator reads

$$Q^\Lambda_{0,\mathbf{k}}(i\omega) = i\omega - f_{1,\mathbf{k}}(\Lambda)\varepsilon_{\mathbf{k}} + \mu - f_2(\Lambda)K(i\omega)$$

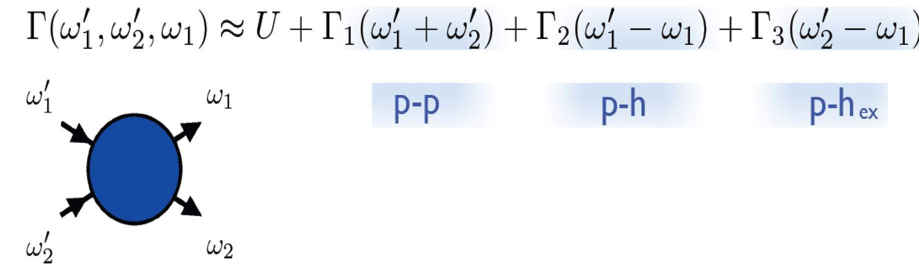
- Same hierarchy of flow equations
- Decouple at fourth order and use initial conditions

$$\Sigma^{\Lambda_{\rm in}}(i\omega) = \Sigma^{\rm DMFT}(i\omega)$$

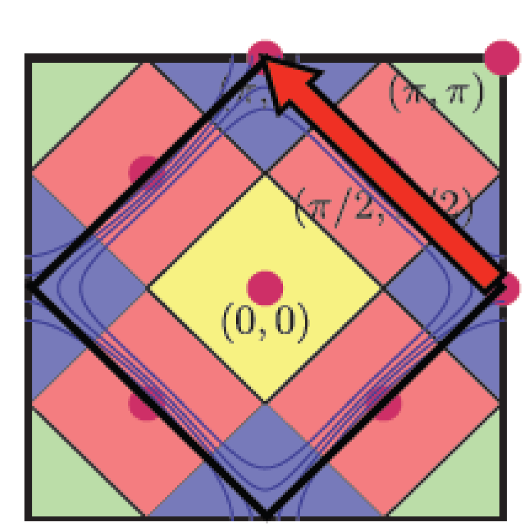
$$\Gamma^{\Lambda_{\rm in}}(i\omega_1', i\omega_2', i\omega_1; \mathbf{k}_1', \mathbf{k}_2', \mathbf{k}_1) = \Gamma^{\rm DMFT}(i\omega_1', i\omega_2', i\omega_1)$$

- Then solve differential equations
- Use channel decomposition

$$\Gamma(\omega_1',\omega_2',\omega_1) \approx U + \Gamma_1(\omega_1'+\omega_2') + \Gamma_2(\omega_1'-\omega_1) + \Gamma_3(\omega_2'-\omega_1)$$



- Momentum patches for vertex functions

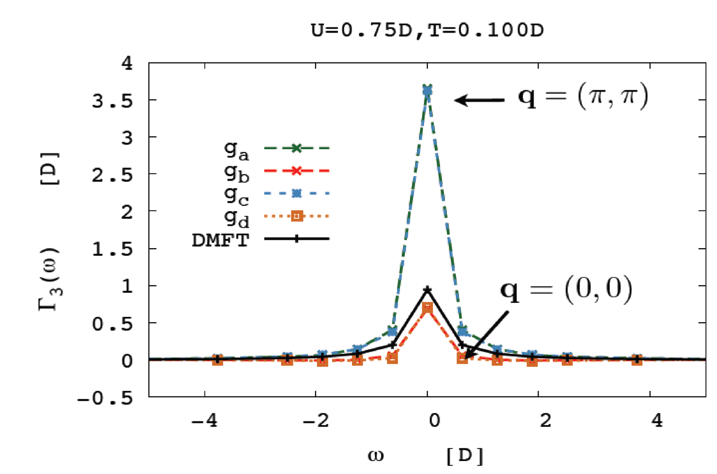


APPLICATION: HUBBARD MODEL

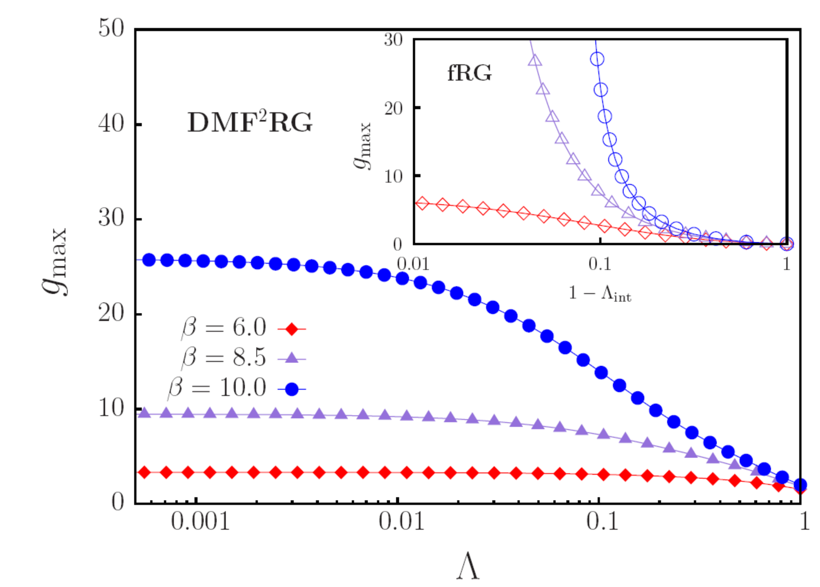
- Study 2d Hubbard model with perfect nesting and strong antiferromagnetic instability [3]

$$H = \sum_{i,j,\sigma}(t_{ij}c^\dagger_{i,\sigma}c_{j,\sigma} + \mathrm{h.c.}) + U\sum_i n_{i,\uparrow}n_{i,\downarrow}$$

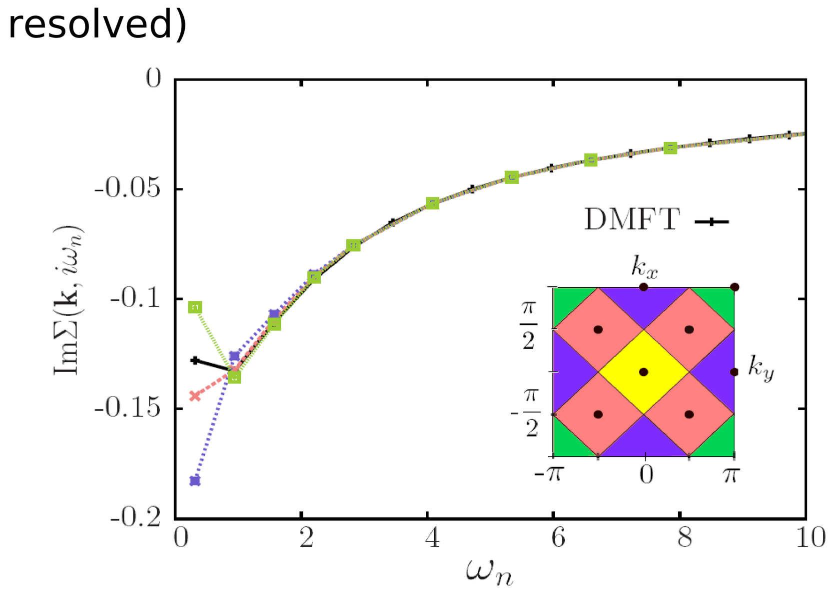
- Vertex function in particle-hole (ex) channel



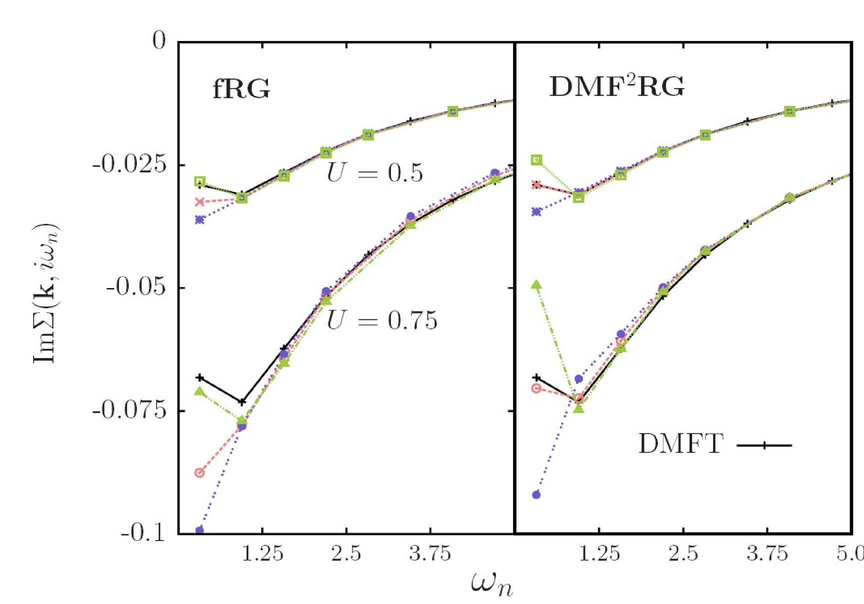
- Flow of vertex functions for different temperatures shows instabilities emerging (comparison with conventional fRG results)



- Results for the self-energy (momentum-resolved)

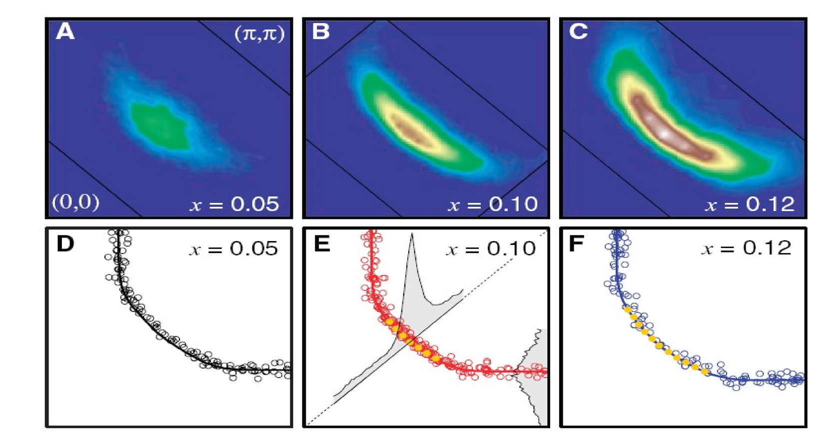


- Comparison with conventional FRG scheme

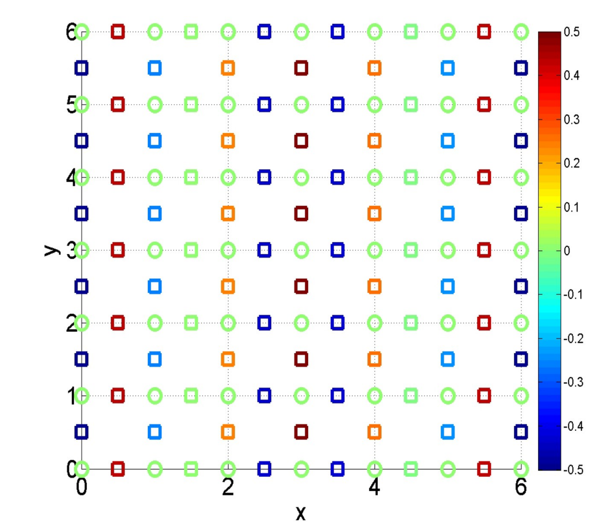


OUTLOOK

- Address Fermi-arc and pseudogap behavior in the cuprates [11]



- Look for charge order in doped Mott insulator [5-7]



CONCLUSIONS

- Proposed a new method combining FRG with DMFT to analyze properties of strongly correlated fermions
- Demonstrate feasibility for 2d Hubbard model at half filling and intermediate coupling
- Many interesting extensions
- Challenge: parameterization of vertex function

LITERATURE

[1] W. Metzner, et. al., Rev. Mod. Phys. (2012)
[2] A. Georges, *et al.*, Rev. Mod. Phys. (1996).
[3] C. Taranto, *et al.*, cond-mat/1307.3475 (PRL '14)
[4] K. Shen, *et al.*, Science 307, 901 (2005)
[5] R. Comin, *et al.*, cond-mat/1402.5415(2014)
[6] K Fujita, *et al.*, cond-mat/1404.0362(2014)
[7] A. Allais, *et al.*, cond-mat/1402.4807 (2014)

ACKNOWLEDGEMENTS

We acknowledge financial support from FWF through the Project No. I-597-N16, (DFG research unit FOR 1346) and I-610-N16, from DFG through research unit FOR 723 and through Grant No. BA 4371/1-1, from RFBR Grant No. 10-02-91003-ANF_a and grant of the Dynasty Foundation, and FWF SFB ViCoM F41.