# Functional RG: from weak to strong coupling in the 2D Hubbard model

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# Outline

## fRG: weak-to-intermediate coupling

- ➡ Frequency dependent interaction
- ➡ Charge divergence
- Self energy and pseudogap

## DMF<sup>2</sup>RG: strong coupling by starting from DMFT solution

- ➡ Local DMFT vertex affects non-local susceptibility
- ➡ *d*-wave pairing fluctuations

Conclusions and outlook







# Outline

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# Motivation: CuO<sub>2</sub> high temperature superconductors



Nature (2015)

#### Phase diagram

Known phases:

- Antiferromagnetism in undoped case
- → d-wave superconductivity for sufficient doping

#### Interest due to:

- Competition of instabilities
- ➡ Strong correlations
- ➡ Quantum criticality

# Prototype: 2D Hubbard model



Zhang and Rice,

- → Low energy model: Cu and O hopping effectively included in t-t' kinetic energy
- Lack of charge instability observed in cuprates

## 2D Hubbard model

$$\mathcal{H} = \sum_{i,j,\sigma} t_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$





• SC d-wave phase in the limit  $U \rightarrow 0$ 

Raghu, Kivelson and Scalapino, PRB (2010)

 $T_c \sim W \exp\left\{-\alpha_2 (t/U)^2 - \alpha_1 (t/U) - \alpha_0\right\} \\ \times \left[1 + \mathcal{O}(U/t)\right]$ 

RG idea:

- Successive rescaling of the effective interaction
- Integrate degrees of freedom following hierarchy of energy scales
- Exact flow from *bare* to the effective action
- Unbiased channel competition (cuprate physics)

Scale dependent propagator:

 $G_0(\mathbf{k}, i\omega) \Rightarrow G_0^{\Lambda}(\mathbf{k}, i\omega)$ 

Equivalence between multi-loop fRG and parquet approx.

Kugler and von Delft, arXiv:1703.06505







Hierarchy of flow equations

Metzner et al. RMP (2012)

Hierarchy of flow equations





ARPES

Comin et al., Science (2013)



#### Metzner et al. RMP (2012)

Fig. 3. Doping dependence of the charge order wavevector  $Q_{\rm CO}$  Data from REXS and STM on Bi2201 [this work and (7)] have represent peak widths, rather than array

Hierarchy of flow equations





ARPES

Comin et al., Science (2013)



spin-wave

- 20

- 15

- 10

(π,0)

Jain et al., Nature (2013)

#### Metzner et al. RMP (2012)

Fig. 3. Doping dependence of the charge order wavevector  $Q_{\rm CO}$  Data from REXS and STM on Bi2201 [this work and (7)] have represent near widths rather than array

Hierarchy of flow equations





ARPES

Comin et al., Science (2013)



Fin. 2. ARPES and theory comparison on Bi2201. Modeled Fermi surface for, on-interacting and (B) the interacting case. which the self-ener  $3\pi/a$  represveen the calcuinodal 3N/<sup>4</sup>/<sup>4</sup>/<sub>0</sub> 

## spin-wave

Jain et al., Nature (2013)



## Metzner et al. RMP (2012)

Fig. 3. Doping dependence of the charge order wavevector  $Q_{\rm CO}$  Data from REXS and STM on Bi2201 [this work and (7)] have represent peak widths, rather than array

Hierarchy of flow equations





ARPES

Comin et al., Science (2013)



Fig. 2. ARPFS and theory comparison on Bi2201. Modeled Fermi surface for, on-interacting and (B) the interacting case, which



## spin-wave

Jain et al., Nature (2013)

 $\begin{array}{c} \bullet \\ \hline \gamma_3^{\Lambda} \\ \hline \gamma_4^{\Lambda} \\ \hline \gamma_4^{\Lambda} \\ \hline \end{array} + \dots$ 

One loop: improper inclusion of soft and amplitude modes

Salmhofer et al., PTP (2004)

#### Metzner et al. RMP (2012)

Fig. 3. Doping dependence of the charge order wavevector  $Q_{\rm CO}$  Data from REXS and STM on Bi2201 [this work and (7)]; here represent pack widths, rather than errors



Full frequency dependent interaction:

$$V^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{1},\boldsymbol{k}_{2},\boldsymbol{k}_{3}) = U -\phi_{sc}^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{1}+\boldsymbol{k}_{2},\boldsymbol{k}_{1},\boldsymbol{k}_{3}) + M^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{3}-\boldsymbol{k}_{1}) + \frac{1}{2}M^{\nu_{1},\nu_{2},\nu_{1}+\nu_{2}-\nu_{3}}(\boldsymbol{k}_{2}-\boldsymbol{k}_{3}) - \frac{1}{2}C^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{2}-\boldsymbol{k}_{3})$$

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Full frequency dependent interaction:

$$V^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{1},\boldsymbol{k}_{2},\boldsymbol{k}_{3}) = U -\phi_{sc}^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{1}+\boldsymbol{k}_{2},\boldsymbol{k}_{1},\boldsymbol{k}_{3}) + M^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{3}-\boldsymbol{k}_{1}) + \frac{1}{2}M^{\nu_{1},\nu_{2},\nu_{1}+\nu_{2}-\nu_{3}}(\boldsymbol{k}_{2}-\boldsymbol{k}_{3}) - \frac{1}{2}C^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{2}-\boldsymbol{k}_{3})$$

Full frequency dependent interaction:

$$V^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{1},\boldsymbol{k}_{2},\boldsymbol{k}_{3}) = U \left(\phi_{sc}^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{1}+\boldsymbol{k}_{2},\boldsymbol{k}_{1},\boldsymbol{k}_{3}) + M^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{3}-\boldsymbol{k}_{1}) + \frac{1}{2}M^{\nu_{1},\nu_{2},\nu_{1}+\nu_{2}-\nu_{3}}(\boldsymbol{k}_{2}-\boldsymbol{k}_{3}) - \frac{1}{2}C^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{2}-\boldsymbol{k}_{3})\right)$$

$$\phi_{SC}^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{Q},\boldsymbol{k}_{1},\boldsymbol{k}_{3}) = S^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{Q}) + d_{\frac{\boldsymbol{Q}}{2}-\boldsymbol{k}_{1}}d_{\frac{\boldsymbol{Q}}{2}-\boldsymbol{k}_{3}}D^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{Q})$$



## Interaction flow and phase diagram

Interaction scheme: (Honerkamp et al., PRB 2004)



DV et al., arXiv: 1708.03539

Critical scale interpreted as critical coupling:  $U_c = \Lambda_c^2 U$ 

- Charge divergence at finite exchange frequency
- Self energy feedback "cures" charge divergence

Consistent with Husemann et al. PRB 2012



## Interaction flow and phase diagram

Interaction scheme: (Honerkamp et al., PRB 2004)



Interaction flow and phase diagram

Dynamic vs static approximation



Magnetic channel



→ Frequency dependence enhances  $1 - \Lambda_c$ 

 The static approximation overestimates the effect of channel competition on the magnetic one

# Effect of frequency dependence on PP d-wave channel



#### d-wave channel affected by two factors:

- ➡ Localized frequency structure Wentzell et al., 2016
- Interaction flow underestimates *d*-wave pairing



DV et al., arXiv: 1708.03539

#### d-wave: dynamic vs static



# Charge divergence

0.20

0.16

 $\mathbf{N}_{\mathrm{c}}$ 



## Self energy suppresses the divergence



# Charge divergence



## What is the origin of the divergence?



### Self energy suppresses the divergence

0.5

# Charge divergence



#### Self energy suppresses the divergence

 $\max(\mathcal{M}^{\Lambda})$ 

 $\max(\mathcal{M}^{\Lambda})$ 

 $\max(-\mathcal{C}^{\Lambda})$ 

0.4

0.5

 $= \max(-\mathcal{C}^{\Lambda})$ 

0.3



# Charge divergence



#### Self energy suppresses the divergence

 $\max(\mathcal{M}^{\Lambda})$ 

 $\max(\mathcal{M}^{\Lambda})$ 

 $\max(-\mathcal{C}^{\Lambda})$ 

0.4

0.5

 $\square \max(-\mathcal{C}^{\Lambda})$ 



# Charge divergence



#### Self energy suppresses the divergence

 $\max(\mathcal{M}^{\Lambda})$ 

 $\max(\mathcal{M}^{\Lambda})$ 

 $\max(-\mathcal{C}^{\Lambda})$ 

0.4

0.5





# Self energy

Self energy in Matsubara axis



- ➡ Almost local along the FS
- → Fermi liquid behaviour even close to iAF instability

#### DV et al., arXiv: 1708.03539

#### Momentum distribution

$$n^{\Lambda}(\mathbf{k}) = 2T \sum_{\nu} \frac{e^{i\nu 0^{+}}}{i\nu - \varepsilon_{\mathbf{k}} + \mu^{\Lambda} - \Lambda \Sigma^{\Lambda}(\mathbf{k}, \nu)}.$$



➡ More broadening in antinodal direction

## Hartree-Fock self energy

Wu, Georges and Ferrero, PRB 2017

Diagrammatics:

Close to magnetic instability  $\mathbf{Q} \simeq (\pi, \pi)$ 

1996

$$-\underbrace{\Sigma^{\Lambda}}_{G_{0}} = \underbrace{\begin{array}{c} \chi_{s} \\ \varphi_{s} \\ G_{0} \end{array}}_{C(\mathbf{k}, i\omega_{n}) \propto \sum_{\mathbf{q}} \sum_{p} \frac{1}{i\omega + i\nu_{p} + \mu - \epsilon_{\mathbf{k}+\mathbf{q}}} \times \frac{1}{(\mathbf{q} - \mathbf{Q})^{2} + \xi^{-2}\nu_{p}/\omega_{\mathrm{sp}} + \xi^{-2}}.$$

$$\underbrace{\begin{array}{c} Ornstein-Zernike \text{ spin} \\ \text{susceptibility: Dare' et al., PRB} \end{array}}_{C(\mathbf{k}, i\omega_{n}) \propto \sum_{\mathbf{q}} \sum_{p} \frac{1}{i\omega + i\nu_{p} + \mu - \epsilon_{\mathbf{k}+\mathbf{q}}} \times \frac{1}{(\mathbf{q} - \mathbf{Q})^{2} + \xi^{-2}\nu_{p}/\omega_{\mathrm{sp}} + \xi^{-2}}.$$

Fock self energy with strong AF fluctuations:

 $\xi >> a$ 

$$\Sigma(\mathbf{k},\omega) = \frac{\Delta^2}{\omega + \mu - \epsilon_{\mathbf{k}+\mathbf{Q}} + i0^+},$$

Pseudogap phase



# Self energy: Fock vs fRG

Fock self energy

0.0

-0.1

-0.2
 -0.3
 -0.3

-0.4

-0.5

0

1









Exact only when the vertex is exact

3

ν

4

2

5

6



Non Fermi-liquid at the hot-spots 

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- ➡ *d*-wave pairing fluctuations

Conclusions and outlook







# DMF<sup>2</sup>RG: flow for the strong coupling

Wentzel et al., PRB 2015

#### Conventional fRG



- Start from bare action: no fluctuations from the beginning
- ➡ Truncation: error accumulated during the flow
- C. Taranto et al., PRL (2014)

Metzner et al. RMP (2012)

## DMF<sup>2</sup>RG: flow for the strong coupling

Wentzel et al., PRB 2015

Extension to strong coupling



$$G_0^{\Lambda_{ini}} = G_{0,R} \neq 0$$

Inclusion of correlation from the beginning

- Reduce truncation error by starting 'closer' to final action
- C. Taranto et al., PRL (2014)







Rohringer et al., PRB (2012)



# DMF<sup>2</sup>RG: strong coupling flow

$$V^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{1},\boldsymbol{k}_{2},\boldsymbol{k}_{3}) = F^{\nu_{1},\nu_{2},\nu_{3}}_{\text{DMFT}} - \phi^{\nu_{1},\nu_{2},\nu_{3}}_{SC}(\boldsymbol{k}_{1} + \boldsymbol{k}_{2},\boldsymbol{k}_{1},\boldsymbol{k}_{3}) + M^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{3} - \boldsymbol{k}_{1})$$
$$+ \frac{1}{2}M^{\nu_{1},\nu_{2},\nu_{1}+\nu_{2}-\nu_{3}}(\boldsymbol{k}_{2} - \boldsymbol{k}_{3}) - \frac{1}{2}C^{\nu_{1},\nu_{2},\nu_{3}}(\boldsymbol{k}_{2} - \boldsymbol{k}_{3})$$

DMF<sup>2</sup>RG: strong coupling flow n = 1 t' = 0  $V^{\nu_1,\nu_2,\nu_3}(k_1,k_2,k_3) = F_{\text{DMFT}}^{\nu_1,\nu_2,\nu_3} - \phi_{SC}^{\nu_1,\nu_2,\nu_3}(k_1+k_2,k_1,k_3) + M^{\nu_1,\nu_2,\nu_3}(k_3-k_1)$  $+ \frac{1}{2}M^{\nu_1,\nu_2,\nu_1+\nu_2-\nu_3}(k_2-k_3) - \frac{1}{2}C^{\nu_1,\nu_2,\nu_3}(k_2-k_3)$ 

Single channel (PHcr) DMF2RG equivalent to ladder-DMFT



➡ Recovery of DMFT Néel temperature only with full frequency dependence

DMF<sup>2</sup>RG: strong coupling flow 
$$n = 1$$
  $t' = 0$   
 $V^{\nu_1,\nu_2,\nu_3}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = F_{\text{DMFT}}^{\nu_1,\nu_2,\nu_3} - \phi_{SC}^{\nu_1,\nu_2,\nu_3}(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1, \mathbf{k}_3) + M^{\nu_1,\nu_2,\nu_3}(\mathbf{k}_3 - \mathbf{k}_1)$   
 $+ \frac{1}{2}M^{\nu_1,\nu_2,\nu_1+\nu_2-\nu_3}(\mathbf{k}_2 - \mathbf{k}_3) - \frac{1}{2}C^{\nu_1,\nu_2,\nu_3}(\mathbf{k}_2 - \mathbf{k}_3)$ 



Strong but localised vertex structure

 ${\bf max} M \sim 10^6$ 

DMF<sup>2</sup>RG: strong coupling flow 
$$n = 1$$
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 $V^{\nu_1,\nu_2,\nu_3}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = F_{\text{DMFT}}^{\nu_1,\nu_2,\nu_3} - \phi_{SC}^{\nu_1,\nu_2,\nu_3}(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1, \mathbf{k}_3) + M^{\nu_1,\nu_2,\nu_3}(\mathbf{k}_3 - \mathbf{k}_1)$   
 $+ \frac{1}{2}M^{\nu_1,\nu_2,\nu_1+\nu_2-\nu_3}(\mathbf{k}_2 - \mathbf{k}_3) - \frac{1}{2}C^{\nu_1,\nu_2,\nu_3}(\mathbf{k}_2 - \mathbf{k}_3)$ 



Spin susceptibility



Strong but localised vertex structure

$$max M \sim 10^6$$

## DMF<sup>2</sup>RG: Néel temperature at half-filling

Spin susceptibility







Brillouin zone

- Mean field critical exponent
- Non-local fluctuations slightly reduce the Néel temperature
- Result stable over a large range of coupling strength

DMF<sup>2</sup>RG: away from half-filling T = 0.08t

Strong coupling regime and doped region





DMF<sup>2</sup>RG: away from half-filling

Strong coupling regime and doped region



No indications for pseudogap: Lack of method or model?  $U = 8t \quad t' = -0.2t$ 

Results:

- Incommensurate antiferromagnetism in undoped case
- Local and Fermi-liquid self-energy as in weak-tointermediate coupling fRG





#### Where the incommensurate peak comes from?

Three possibilities:

- ★ From the *non-locality* of the self-energy?
- $\star$  From the channel competition?
- ✓ From the DMFT vertex?

$$\chi_0^s = -T \sum_{\nu} \int_{\boldsymbol{k}} G_{\boldsymbol{k},\omega} G_{\boldsymbol{Q}+\boldsymbol{k},\omega+\nu}$$

with 
$$\Sigma = \Sigma_{\text{DMFT}}$$







Matrix multiplication in frequency space



Local vertex affects non-local spin susceptibility

DMF<sup>2</sup>RG: *d*-wave pairing fluctuations

Lowering the temperature:







0 V 1

-1

- → Strong *d*-wave pairing fluctuations in the iAF phase
- → Localised frequency structure as in fRG
- → Precursor of *d*-wave instability at lower  $T_c$ ?

# Conclusion

- Important frequency dependence in the intermediate coupling
- Presence of charge divergence, explained by RPA-like formulae and suppressed by self energy feedback
- ➡ Flow to the strong coupling by starting from DMFT solution
- Local vertex affects non-local susceptibility
- Strong *d*-wave pairing fluctuations at Temperature studied

# Outlook

Lowering the Temperature to enhance the interplay between AF and SC



 $\mathcal{M}^{\Lambda_c}$ ,  $\mathbf{Q} = (\pi, \pi - \delta)$ ,  $\Omega = 0$ 





# Questions?



Thank you for your attention

## Charge divergence: perpendicular ladder

RPA-like magnetic fluctuations

$$U_{\mathbf{Q},\Omega}^{\text{eff}} = \frac{U}{1 - U \Pi_{\mathbf{Q},\Omega}} = \mathbf{O} + \mathbf{$$

RPA-like charge fluctuations (generated by magnons)

$$\tilde{\mathcal{C}}_{\mathbf{Q},\Omega}(\nu_1,\nu_3) = U_{\nu_1-\nu_3}^{\text{eff}} \left[ \delta_{\nu_1,\nu_3} + U_{\nu_1-\nu_3}^{\text{eff}} \Pi_{\mathbf{Q},\Omega}(\nu_1) \right]_{\prime}^{-1} = \underbrace{\phantom{\sum}}_{\prime} + \underbrace{\phantom{\sum}}_{$$

→ Bosonic frequency  $\Omega = \nu_2 - \nu_3$  enters only in the (not summed) bubble

Frequency dependent bubble

$$\Pi_{\mathbf{Q},\Omega}(\nu) = -\int_{\mathbf{p}} G_0(\mathbf{p},\nu) G_0(\mathbf{p}+\mathbf{Q},\nu+\Omega).$$

Similar to FLEX approx.

## Charge divergence: perpendicular ladder

$$\tilde{\mathcal{C}}_{\mathbf{Q},\Omega}(\nu_{1},\nu_{3}) = U_{\nu_{1}-\nu_{3}}^{\text{eff}} \left[ \delta_{\nu_{1},\nu_{3}} + U_{\nu_{1}-\nu_{3}}^{\text{eff}} \Pi_{\mathbf{Q},\Omega}(\nu_{1}) \right]_{\ell}^{-1} \qquad \Pi_{\mathbf{Q},\Omega}(\nu) = -\int_{\mathbf{p}} G_{0}(\mathbf{p},\nu) G_{0}(\mathbf{p}+\mathbf{Q},\nu+\Omega).$$



- ➡ Same structure appearing in full fRG
- Divergent when lowering the temperature
- Qualitative but not quantitative picture

Property of the bubble:

$$T\sum_{\nu} \Pi_{\mathbf{Q}\to(0,0),\Omega}(\nu) = C\delta_{\Omega,0},$$

fRG: the self energy feedback cures the divergence