

# **Truncated Unity Functional renormalization group** (TUfRG) for 2D lattices: getting more quantitative

- 1. fRG: quantitative issues
- 2. TUfRG in momentum space: recent results
- 3. TUfRG for frquency dependence: outlook

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## **Functional RG for Hubbard-type models**

#### Model bandwidth $\Lambda$ Interaction at scale $H_{\text{int}} = U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + V_1 \sum_{\langle i,j\rangle,s,s'} n_{i,s} n_{j,s'}$ bandwidth ~ eV (few eVs) not much structure, + $V_2 \sum_{\langle \langle i,j \rangle \rangle, s,s'} n_{i,s} n_{j,s'} + V_3 \sum_{\langle \langle \langle i,j \rangle \rangle \rangle, s,s'} n_{i,s} n_{j,s'}$ mean-field decoupling ambiguous/impossible ambiguous/impossible functional Intermediate energy scales: particle-hole pairs, particle-particle loop corrections generate structure renormalization group (fRG): lower $\Lambda$ in effective low-energy interaction $V_{\Lambda}(K_{1}, K_{2}, K_{3})$ $\begin{array}{c|c} 10\text{-}100 \ meV \\ \ge T_c \end{array} \quad H_{\text{eff}} = \frac{1}{2} \sum_{\vec{p}, \vec{p'}, \vec{q}} V(\vec{p}, \vec{p'}, \vec{p} + \vec{q}) \ c^{\dagger}_{\vec{p} + \vec{q}, s} c^{\dagger}_{\vec{p'} - \vec{q}, s'} c_{\vec{p'}, s'} c_{\vec{p}, s} \qquad \underset{\mathsf{k}_2 \\ \end{array} \\ \begin{array}{c} \mathsf{k}_2 \\ \mathsf{k}_4 \end{array} \end{array}$ $\Rightarrow$ e.g. guided mean-field decoupling 0

Functional Renormalization Group (fRG):

Provides low-energy effective action & momentum structure  $V_{\Lambda}(k,k',k+q)$ ! Removes ambiguities of mean-field decouplings.

# **Functional RG**



Keep track of wavevector structure: *N***-patch** 

- Discretize Brillouin zone into *N* patches
- More recently: channel decomposition & form factor expansion

Often neglected: self-energy, higher-order interactions, frequency dependence



# Flow to strong coupling

Standard cases without self-energy feedback: Flow to strong coupling





Leading low-energy correlations Energy scales →'Weather forecast'

> Metzner, Salmhofer et al. RMP 2012

# **1. Quantitative issues: testing fRG for materials**

Take model Hamiltonian with parameters given, e.g., by DFT & cRPA



#### Can fRG become quantitative low-energy frontend of ab-initio theory?

Besides groundstate: Energy scales for phase transitions & relevant excitations? Trends within material families?

# Trends in 1111 iron arsenide superconductors



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Iron-Based Layered Superconductor La[O<sub>1-x</sub>F<sub>x</sub>]FeAs (x = 0.05-0.12) with  $T_c = 26$  K

Yoichi Kamihara,\*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§





Table I. Maximum  $T_c$  in each  $RFeAs(O_{1-x}F_x)$ . The F concentration x, which gives the maximum  $T_c$  is shown.  $T_c^{Max}$  is determined at the onset temperature of superconducting transition in resistivity measurements.

	R									
	La	Ce	Pr	Nd	Sm	Gd	Tb	Dy		
$T_{\rm c}^{\rm Max}$ (K)	28	41	52	52	55	36	46	45		
x	0.11	0.16	0.11	0.11	0.1	0.17	0.1	0.1		

Ishida, K., Nakaii, Y. & Hosono, H. To what extent iron-pnictide new superconductors have been clarified: A progress report. *J. Phys. Soc. Jpn* **78**, 062001 (2009).

Z.-A. Ren, W. Lu, J. Yang, W. Yi, X.-L. Shen, Z.-C. Li, G.-C. Che, X.-L. Dong, L.-L. Sun, F. Zhou, and Z.-X. Zhao: Chin. Phys. Lett. **25** (2008) 2215.

## La-1111 versus Sm-1111

Why is  $T_c$  in La-1111 much lower than in Sm-1111?



# Trends in 1111 iron arsenides

fRG for 8-band model reproduces sizable  $T_c$ -difference for pairing, while keeping AF-SDW scale unchanged





# **Model for layered graphene**

E.g. AB (bernal) stacked bilayer:

$$\begin{split} H_l^{\parallel} &= -t \sum_{\sigma, \vec{R}, \vec{\delta}_i} \left( b_{l,\sigma}^{\dagger} (\vec{R} + (-)^{l-1} \vec{\delta}_i) a_{l,\sigma}(\vec{R}) + \text{h.c.} \right) \\ H^{\perp} &= -t_{\perp} \sum_{\sigma, \vec{R}} \left( a_{1,\sigma}^{\dagger}(\vec{R}) a_{2,\sigma}(\vec{R}) + \text{h.c.} \right) \end{split}$$

eV

0.6 0.4

0.2

-0.2-0.4-0.6

Four bands, 2 quadratic band crossing points @ *K*,*K*'



Take ab-initio-derived interaction parameters ('constrained RPA'), interpolate between mono-layer and graphite values

	Graj	phene	Graphite		
	Bare	cRPA	Bare	cRPA	
$U_{00}^{A \text{ or } B}$ (eV)	17.0	9.3	17.5, 17.7	8.0, 8.1	
$U_{01}^{00}$ (eV)	8.5	5.5	8.6	3.9	
$U_{02}^{A \text{ or } B}$ (eV)	5.4	4.1	5.4, 5.4	2.4, 2.4	
$U_{03}^{02}$ (eV)	4.7	3.6	4.7	1.9	

Wehling et al. PRL 2011

# N-Layer graphene @ charge neutrality



# The 'scale challenge'

**fRG scales for gaps** in layered graphene seems **far too large** compared to experiment, even with 'realistic' model parameters Sources of error:



Model incorrect? Other interactions? Long-range Coulomb!

Model parameters incorrect? cfRG instead of cRPA?

# **Resolve patching ambiguities**



Daniel D. Scherer, Michael M. Scherer, C. Honerkamp, Phys. Rev. B 92 (2015)



# 2. Truncated unity fRG in momentum space

- Builds on channel decomposition à la Salmhofer et al. (Husemann, Salmhofer, PRB 2009)
- Incorporates numerical advantages of singular-mode (SM-)fRG, Q.H. Wang et al. PRB 21012
- Idea: insert resolutions of unity in momentum space factor basis into one-loop RG eqns



$$\delta_{kk'} = \frac{1}{N} \sum_{x} e^{i(k-k')x}$$

J. Lichtenstein, D. Sanchez dIP, D. Rohe, CH, S.A. Maier Computer Physics Communications 2017

- Truncation of basis provides physically transparent approximation & high momentum resolution
- Parallelizes nicely on high-performance architectures (= headroom for attacking frequency-dependence, selfenergies, …)



# **Channel decomposition**

Husemann, Salmhofer, Giering, Eberlein & Metzner , Maier & CH ... Karrasch et al.

Instead of one function of three variables, use three functions *P,D, C* of **one 'strong/bosonic' variable** 

 $s = k_1 + k_2$ ,  $t = k_3 - k_1$ ,  $u = k_4 - k_1$ 



#### Form factor basis: $P_{\Lambda}(k_1, k_3; s) = \sum f_{x_1}(k_1) f_{x_3}^*(k_3) P_{\Lambda}(x_1, x_3; s)$ $x_1, x_3$ $x_i = \vec{b}_i$ bonds on real space lattice Form factors/basis functions $f_n(\mathbf{k})$ most easily organized on real space Bravais lattice spanned by bond vectors real lattice $\bigcirc$ $\bigcirc$ $\bigcirc$ $\bigcirc$ $\bigcirc$ $f_{\vec{b}}(\vec{r}) = \delta_{\vec{r},\vec{b}}$ bond functions $\bigcirc \bigcirc \bigcirc \bigcirc \bigcirc$ Symmetrize wrt IRREPs of point group G reciprocal lattice

 $f_{l}(\vec{r}) = \sum_{R \in \mathcal{G}} a_{l}(R) \delta_{\vec{r},R\vec{b}}$ e.g. 'd-wave'  $\bigcirc \bigcirc \bigcirc \frown \bigcirc + \bigcirc \frown \bigcirc \frown \bigcirc$ 

For most cases: Short bonds **b** most important <=> form factors  $f_n(\mathbf{k})$  smooth  $\begin{aligned} \mathbf{reciprocal lattice} \\ f_{\vec{b}}(\vec{k}) &= e^{i\vec{k}\cdot\vec{b}} \\ \mathbf{b} \\ f_{\vec{b}}(\vec{k}) &= e^{i\vec{k}\cdot\vec{b}} \\ f_{l}(\vec{k}) &= \sum_{R \in \mathcal{G}} a_{l}(R) f_{R\vec{b}}(\vec{k}) \\ f_{d_{x^{2}-y^{2}}}(\vec{k}) \propto \cos k_{x} - \cos k_{y} \end{aligned}$ 

C. Platt, W. Hanke, R. Thomale, Adv. Phys. 2013

## **Fermion bilinear interaction**



In real space, *P*-interaction becomes pair-pair scattering:

$$H_{V} = \frac{1}{2} \sum_{\substack{l_{1}, l_{3} \\ s, s'}} \left[ \sum_{\vec{b}_{3}} a_{l_{3}}^{*}(\vec{b}_{3}) c_{\vec{r}_{3}, s}^{\dagger} c_{\vec{r}_{3} + \vec{b}_{3}, s'}^{\dagger} \right] V_{l_{1}, l_{3}}^{P} \begin{pmatrix} \vec{r}_{1} - \vec{r}_{3} + \frac{\vec{b}_{1} - \vec{b}_{3}}{2} \end{pmatrix} \begin{bmatrix} \sum_{\vec{b}_{1}} a_{l_{1}}(\vec{b}_{1}) c_{\vec{r}_{1} + \vec{b}, s'} c_{\vec{r}_{1}, s} \\ \text{incoming pair, short ranged} \end{bmatrix}$$
  
outgoing pair, short ranged pair distance, can get long ~ exchange boson  
 $\vec{r}_{3}$  Channel decomposition is way of rewriting full interaction as sum of interactions between all possible/necessary fermion bilinears! particle-hole-pairs

$$\begin{array}{cccc} \text{particle-particle-particle-pairs} & \text{particle-hole-pairs} \\ \text{pairs} & \downarrow & \text{particle-hole-pairs} \\ V_{\Lambda}(k_1, k_2, k_3) = V_0(k_1, k_2, k_3) + P_{\Lambda}(k_1, k_3; s) + D_{\Lambda}(k_1, k_4; t) + C_{\Lambda}(k_1, k_3; u) \end{array}$$

no spin flip

Intuitive representation with meaningful truncations

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# **Numerically still hard**



 $V_{\Lambda}(k_1, k_2, k_3) = V_0(k_1, k_2, k_3) + P_{\Lambda}(k_1, k_3; s) + D_{\Lambda}(k_1, k_4; t) + C_{\Lambda}(k_1, k_3; u)$ 

(other channels similar)

# **Truncated unity fRG: matrix flow equations**

Consider flow of pairing interaction

$$\dot{P}_{\Lambda}(k_1, k_3; s) = \frac{T}{N_L} \sum_k V_{\Lambda}(k_1, k; s) L_{\rm PP}(k; s) V_{\Lambda}(k, k_3; s)$$

Insert (truncated) unities: /

 $\dot{P}_{\Lambda}$ 

$$V_{\Lambda}(k_{1},k;s) = \sum_{k'} \delta_{k,k'} V_{\Lambda}(k_{1},k';s) = \frac{1}{N} \sum_{x'} e^{ikx'} \sum_{k'} e^{-ik'x'} V_{\Lambda}(k_{1},k';s)$$
$$(k_{1},k_{3};s) = \sum_{x',x''} \left[ \frac{1}{N} \sum_{k'} V_{\Lambda}(k_{1},k';s) e^{-ik'x'} \right] \cdot \left[ \frac{T}{N_{L}} \sum_{k} e^{ik(x'-x'')} L_{PP}(k;s) \right] \cdot \left[ \frac{1}{N} \sum_{k''} e^{ik''x''} V_{\Lambda}(k'',k_{3};s) \right]$$

Project both sides on form factor basis:  $\dot{P}_{\Lambda}(x_1, x_3; s) = \frac{1}{N} \sum_{k_1, k_3} e^{ik_1x_1} \dot{P}_{\Lambda}(k_1, k_3; s) e^{-ik_3x_3}$ 

$$\Rightarrow \dot{P}_{\Lambda}(x_1, x_3; s) = \frac{1}{N} \sum_{x', x''} P[V]_{\Lambda}(x_1, x'; s) L_{PP}(x', x''; s) P[V]_{\Lambda}(x'', x_3; s)$$

Flow eqns become matrix products of projected couplings and loops (no slow integrals)

$$L_{\rm PP}(x',x'';s) = \frac{T}{N_L} \sum_{k} e^{ik(x'-x'')} L_{\rm PP}(k;s)$$

S. Maier

Truncate sum, only

factors, bonds |x|<R

take relevant form

 $\delta_{kk'} = \frac{1}{N} \sum e^{i(k-k')x}$ 

# How does well it work?

J. Lichtenstein, D. Sanchez dlP, D. Rohe, CH, S.A. Maier Computer Physics Communications 2017

#### Phases and convergence in *t*-*t*<sup>·</sup> Hubbard model



Look at momentum-resolved response function (beyond RPA) Include long-range Coulomb interactions

# **Response functions beyond RPA**

High momentum resolution for 'bosonic' variables (~6000 1 points) permits study of response functions beyond RPA

Peaks of C-channel (=spin channel) at van Hove  $filling_{\gamma}^{k}$  for different *t*':

TUfRG has weaker **peak splitting** than random phase approximation (RPA)







J. Lichtenstein, S.A. Maier, D. Sanchez de la Pena, D. Rohe, CH, CPC 2017

# 3. TUfRG for frequencies: Why?

 Width Ω of interactions on frequency axis matters for critical scales, see e.g. BCS



w/o frequency dependence, as previous fRG ( $\Omega = \infty$ )





# Frequency structure of phonon-mediated<br/>interaction $V_{ph-med.}(\omega_1, \omega_3) = V_0 \frac{\Omega^2}{(\omega_1 - \omega_3)^2 + \Omega^2}$



# Critical scales with frequency dependence, for spin-fluctuation pairing, the hard way

- For spin-fluctuation-mediated pairing:  $\Omega = \Omega_{sf}$  (~ mass of spin fluctuations)
- Simple two-patch model (= toy model for spin-fluctuation pairing), interactions depending on three Matsubara frequencies



#### **Frequency basis**

Label frequency basis function by imaginary time  $t \in [0,\beta]$ 

$$f_{\tau}(i\omega_{n}) = \frac{1}{\sqrt{\beta}} e^{i\omega_{n}\tau} \qquad \tau_{l} = l\Delta\tau \qquad \text{with} \quad l \in 0, \dots N_{\tau} - 1 \quad \text{and} \quad \Delta\tau = \frac{\beta}{N_{\tau}}$$

$$\implies \text{sampling rate } f_{s} = 1/\Delta\tau = N_{\tau}/\beta \qquad \omega_{\max} = 2\pi \cdot \frac{f_{s}}{2} = N_{\tau}\pi T$$
Matrix elements
phonon propagator
$$D_{\tau,\tau'}(\tau_{m}) = \frac{1}{\sqrt{N_{\tau}}} \sum_{\nu} \delta_{l,0}\delta_{l',0}N_{\tau}D_{0} \frac{\Omega^{2}}{\nu^{2} + \Omega^{2}} e^{-i\nu\tau_{m}}$$

$$= \beta\delta_{\tau,0}\delta_{\tau',0}\sqrt{N_{\tau}}\frac{D_{0}\Omega}{2} n_{B}(\Omega) \left\{ e^{\Omega\tau_{m}} + e^{-\Omega\tau_{m}}e^{\beta\Omega} \right\}$$
Phonon propagator
projected on P channel
$$P_{\tau,\tau'}(s) \left[ V^{(D_{0,0})} \right] = \delta_{\tau,\tau'} \beta \frac{D_{0}\Omega}{2} n_{B}(\Omega) \left\{ e^{\Omega\tau_{l}} + e^{-\Omega(\tau_{l}-\beta)} \right\}$$
P channel flow equation
$$\frac{d}{d\Lambda} P_{\Lambda}(\tau,\tau';s) = N_{\tau}^{-1} \sum_{\tau'',\tau'''} P_{\Lambda}(\tau,\tau'';s) \dot{L}_{\text{PP}}^{\Lambda}(\tau'',\tau''';s) P_{\Lambda}(\tau''',\tau';s)$$

Projected bubble

$$L_{\rm PP}^{\epsilon,\epsilon'}(\tau,\tau';s) = T \sum_{\omega_n} \frac{1}{i\omega - \epsilon} \frac{1}{-i\omega + is - \epsilon'} e^{i\omega_n(\tau_l - \tau')}$$
$$= \frac{1}{-is + \epsilon + \epsilon'} \left\{ [1 - n_F(\epsilon')] e^{is|\tau - \tau'|} e^{-\epsilon'|\tau - \tau'|} - n_F(\epsilon) e^{\epsilon|\tau - \tau'|} \right\}$$

## **Critical scales in BCS model**

TUfRG with frequency basis: test for phonon-mediated pairing





# Conclusions

- Functional RG is a versatile tool to explore low-energy physics of interacting fermions in low dimension, for material studies qualitatively useful (see R. Thomale)
- Quantitative precision is currently improved
- Wavevector-TUfRG allows to reach high resolution and convergence wrt to form factor basis
- Frequency-TUfRG should work as well …



Table I. Maximum  $T_c$  in each RFeAs( $O_{1-x}F_x$ ). The F concentration x, which gives the maximum  $T_c$  is shown.  $T_c^{Max}$  is determined at the onset temperature of superconducting transition in resistivity measurements.



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Z-A. Ren, W. Lu, J. Yang, W. Yi, X.-L. Shen, Z.-C. Li, G.-C. Che, X.-L. Done, L.-J. Sun, F. Zhou, and Z.-X. Zhao: Chin. Phys. Lett. 25

(2008) 2215



