

Detecting a preformed pair phase: The response to a pairing forcing field

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FWF

Der Wissenschaftsfonds.

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New Generation in Strongly Correlated Electron Systems

Trogir, September 14, 2015

1 Introduction: Physics of the Pseudogap

Cuprates phase diagram

Experimental and Theoretical evidences of the pseudogap: **performed pair physics ?**

2 Tools: Attractive Hubbard model and dynamical mean field theory

The Hubbard model and the pairing coupling

Dynamical Mean-Field Theory (DMFT)

3 Work and Results

DMFT results under a **pairing forcing field** : the superconducting response

Physical understanding: **Atomic limit**

Physical understanding: **Two-sites model**

Interpretation of DCA results: cuprates physics

4 Conclusions and Outlook

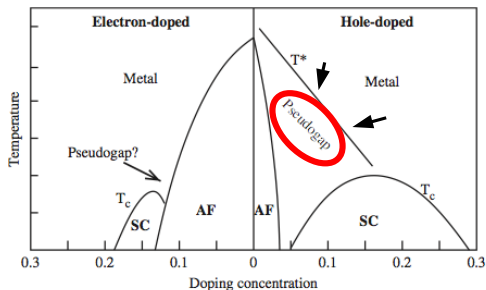
Introduction: Physics of the Pseudogap

Cuprates phase diagram and the pseudogap investigation

Pseudogap physics in high- T_c superconductors

High- T_c superconductors

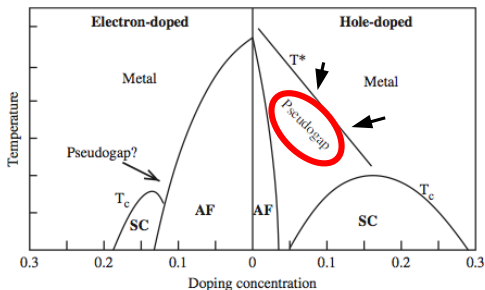
J. G. Bednorz and K. A. Müller, *Z. Phys. B Condens. Matter*
(1986)



Pseudogap physics in high- T_c superconductors

High- T_c superconductors

J. G. Bednorz and K. A. Müller, *Z. Phys. B Condens. Matter*
(1986)



Main features of the **Pseudogap**:

- **Suppression** of spectral weight at Fermi level \rightarrow observed in spectra (ARPES, optics..) and thermodynamics (NMR)
- charge and spin pattern, but **no** clear signatures of long range **order**

Several techniques available

NMR

ARPES

STM

...

Pump-probe spectroscopy

[A. Cavalleri *Phys. Rev. B* (2014), F. Cilento *Nat. Commun.* (2014)]

Experimental evidences

Several techniques available

NMR

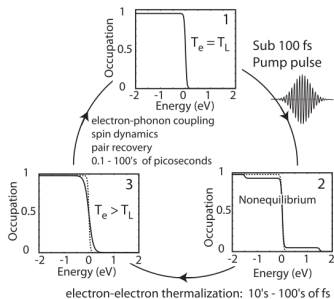
ARPES

STM

...

Pump-probe spectroscopy

[A. Cavalleri *Phys. Rev. B* (2014), F. Cilento *Nat. Commun.* (2014)]



Manipulation of the **Pseudogap**
to trigger new thermodynamic phase
PG \Rightarrow **SC** (or a more conducting metal?)

Debate on the pseudogap physics

Competing-order scenario

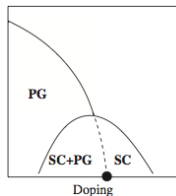
- Weak-coupling theories

[D. J. Scalapino *Rev. Mod. Phys.* (2012)]

- Spin Fluctuations

[B. Kyung *Phys. Rev. B* (2006)]

- ...



Preformed-pair scenario $\rightarrow |\Delta| \neq 0 \langle \Delta \rangle = 0$

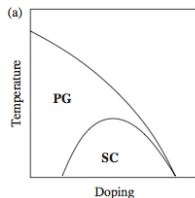
- RVB

[P.W. Anderson, *Science* (1987)]

- BCS-BEC crossover physics

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- ...



Debate on the pseudogap physics

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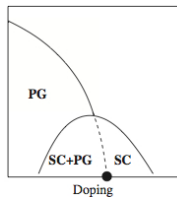
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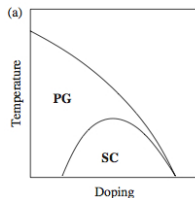
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- ...



Aim of the work

Set a solid **test-bed** to detect the presence of **preformed pairs**

Tools

Hubbard model and dynamical mean field theory

Our basic model

The Hubbard model

Hubbard model:

$$H = \underbrace{-t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.)}_{H_{\text{kin}}} + U \underbrace{\sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right)}_{H_U} \Rightarrow \text{Half-filling}$$

Attractive ($U < 0$)



s-wave **SC** + **CDW**

Mapping



Repulsive ($U > 0$)



AFM

Our basic model

Test-bed model

..Response to a **pairing forcing field** η :

$$H = \underbrace{-t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.)}_{H_{kin}} + \underbrace{U \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right)}_{H_U} - \underbrace{\eta \sum_i (c_{i\downarrow} c_{i\uparrow} + h.c.)}_{H_\eta}$$

Attractive ($U < 0$)

s-wave **SC** + **CDW**

Mapping
 \longleftrightarrow

Repulsive ($U > 0$)

AFM

Pairing coupling

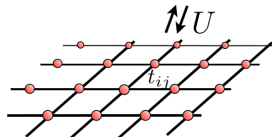
Preformed pairs
couple with η



Magnetic moments **do not**
couple with η



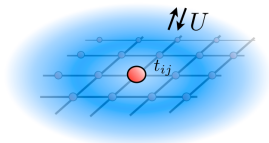
Tool: Dynamical Mean-Field Theory



Exact solutions only available
in **one** and **infinite** dimensions
($d \rightarrow \infty$)

See previous lecture by Jan Tomczak

Tool: Dynamical Mean-Field Theory



[W. Metzner and D. Vollhard *Phys. Rev. Lett.* (1992)]

[A. Georges and G. Kotliar *Phys. Rev. B* (1996)]

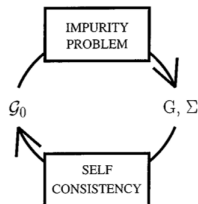
See previous lecture by Jan Tomczak

Approximation:

Looking at the lattice
in a **MF**-fashion
by an **effective bath**

MFT \rightarrow **No** correlations

DMFT \rightarrow **No spatial** correlations
Yes temporal correlations



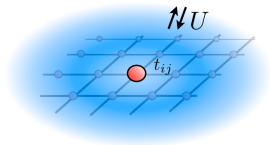
Self-Consistency

$$\mathcal{G}_0(i\omega_n)^{-1} = i\omega_n + \mu + G(i\omega_n)^{-1} - R[G(i\omega_n)]$$

$$G(\tau - \tau') = -\langle Tc(\tau)c^\dagger(\tau') \rangle_{S_{\text{eff}}} \quad \Sigma(i\omega_n) = \mathcal{G}_0(i\omega_n)^{-1} - G(i\omega_n)^{-1}$$

Auxiliary Problem: Anderson Impurity Model (AIM)

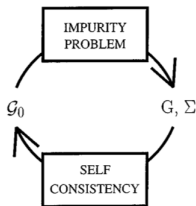
Tool: Dynamical Mean-Field Theory



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Approximation:

Looking at the lattice
in a **MF**-fashion
by an **effective bath**

MFT \rightarrow **No** correlations

DMFT \rightarrow **No spatial** correlations
Yes temporal correlations

Broken Symmetry:

Matrix in the Nambu formalism
Self-Consistency

$$\hat{G}_0(i\omega_n)^{-1} = i\omega_n \hat{\tau}_0 + \mu \hat{\tau}_3 - t^2 \hat{\tau}_3 \hat{G}(i\omega_n) \hat{\tau}_3$$

Bethe Lattice

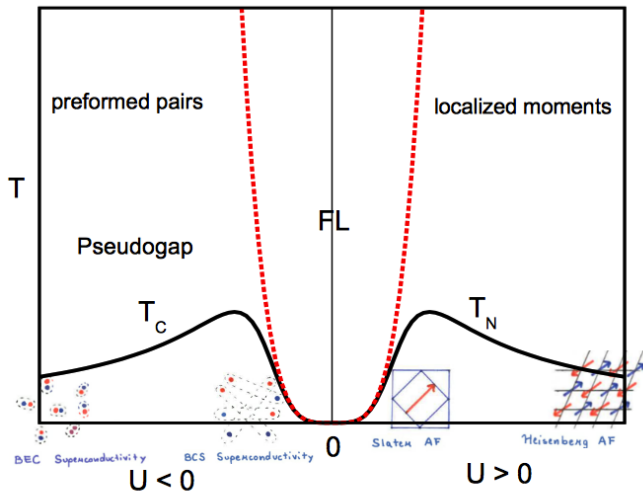
Auxiliary Problem: Superconducting Anderson Impurity Model (AIM)

Work and Results

DMFT results under a pairing forcing field:
the superconducting response

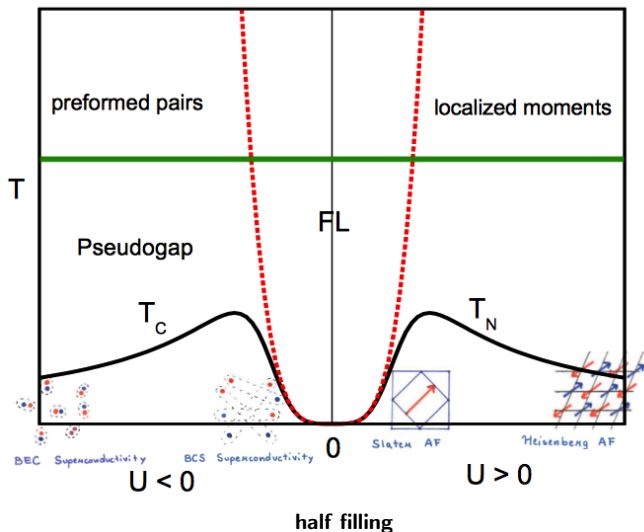
Detecting preformed pairs

Attractive and Repulsive Hubbard model: the phase diagram



Detecting preformed pairs

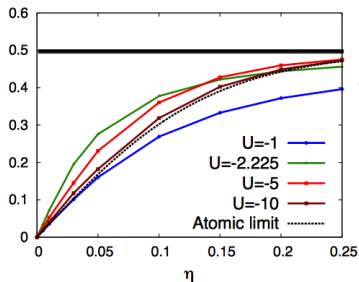
Attractive and Repulsive Hubbard model: the phase diagram



DMFT results under a forcing pairing field

$$H = H_{\text{kin}} + H_U - \underbrace{\eta \sum_i (c_{i\downarrow} c_{i\uparrow} + \text{h.c.})}_{H_\eta} \quad \Rightarrow \quad \Delta(\eta) = \frac{1}{N} \sum_i \langle c_{i\downarrow} c_{i\uparrow} \rangle$$

Attractive



Regime Value

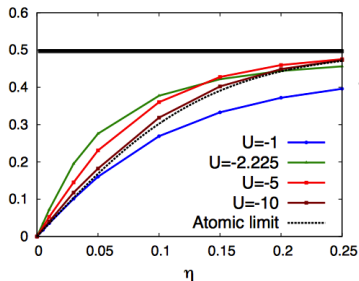
$$\langle c_{i\downarrow} c_{i\uparrow} \rangle \xrightarrow{\eta \rightarrow \infty} \frac{1}{2}$$

$$\beta = \frac{1}{k_B T} = 7D^{-1}$$

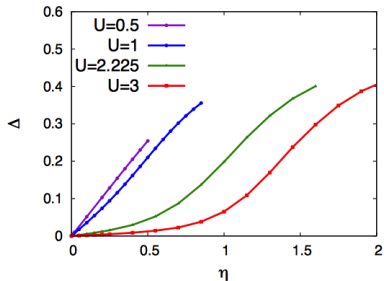
DMFT results under a forcing pairing field

$$H = H_{\text{kin}} + H_U - \eta \underbrace{\sum_i (c_{i\downarrow} c_{i\uparrow} + \text{h.c.})}_{H_\eta} \quad \Rightarrow \quad \Delta(\eta) = \frac{1}{N} \sum_i \langle c_{i\downarrow} c_{i\uparrow} \rangle$$

Attractive



Repulsive

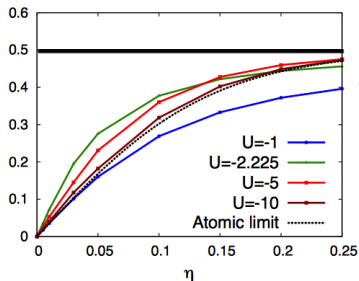


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DMFT results under a forcing pairing field

$$H = H_{\text{kin}} + H_U - \underbrace{\eta \sum_i (c_{i\downarrow} c_{i\uparrow} + \text{h.c.})}_{H_\eta} \Rightarrow \Delta(\eta) = \frac{1}{N} \sum_i \langle c_{i\downarrow} c_{i\uparrow} \rangle$$

Attractive



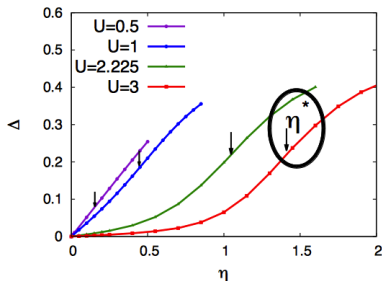
$$\frac{\partial^2 \Delta(\eta)}{\partial \eta^2} < 0$$

$$\beta = \frac{1}{k_B T} = 7D^{-1}$$

Regime Value

$$\langle c_{i\downarrow} c_{i\uparrow} \rangle \xrightarrow{\eta \rightarrow \infty} \frac{1}{2}$$

Repulsive

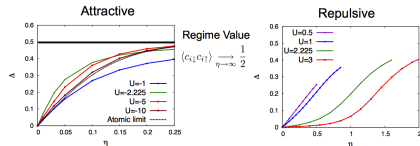


$$\frac{\partial^2 \Delta(\eta)}{\partial \eta^2} > 0 \quad \eta \in [0, \eta^*]$$

Interpretation

Highlights of the results

- **Suppression** of the **linear response** for $U > 0$
- **Positive second derivative** \nrightarrow **absence** of preformed pairs



Physical interpretation

$$\Delta(\eta) = \Delta(\bar{\eta}) + \left. \frac{\partial \Delta}{\partial \eta} \right|_{\bar{\eta}} (\eta - \bar{\eta}) + \left. \frac{\partial^2 \Delta}{\partial \eta^2} \right|_{\bar{\eta}} (\eta - \bar{\eta})^2 + \dots$$

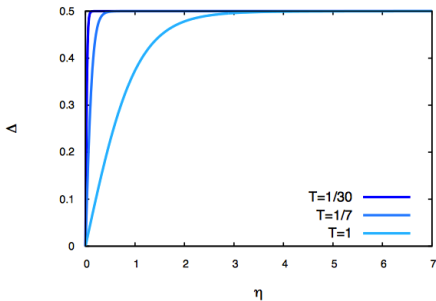
- $\left. \Delta(\bar{\eta}) \right|_{\bar{\eta}=0} = 0$ above the critical temperature;
- $\chi_{\Delta} = \left. \frac{\partial \Delta}{\partial \eta} \right|_{\bar{\eta}=0} \rightarrow$ Fluctuation-Dissipation theorem
- $\left. \frac{\partial^2 \Delta}{\partial \eta^2} \right|_{\bar{\eta}} \rightarrow$ **physical meaning?**

Why is the second derivative sensitive to preformed pairs?

Atomic limit

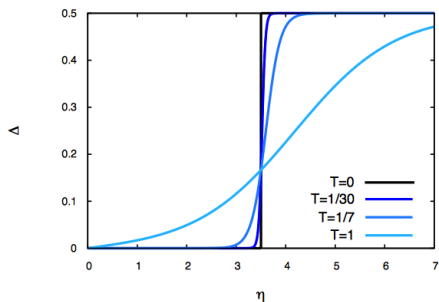
Attractive $U < 0$

$$\Delta_{att}^{hf}(\eta) = \frac{1}{2} \frac{\sinh(\beta\eta)}{\cosh(\beta\eta) + e^{-\beta\frac{|U|}{2}}}$$



Repulsive $U > 0$

$$\Delta_{rep}^{hf}(\eta) = \frac{1}{2} \frac{\sinh(\beta\eta)}{\cosh(\beta\eta) + e^{\beta\frac{U}{2}}}$$



$$n_s = 5$$

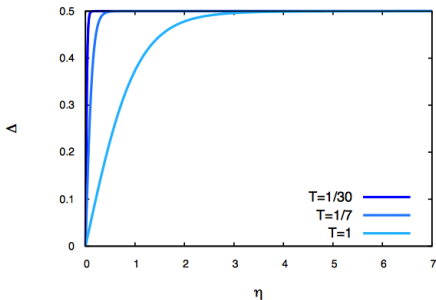
$$|U| = 7D$$

Why is the second derivative sensitive to preformed pairs?

Atomic limit

Attractive $U < 0$

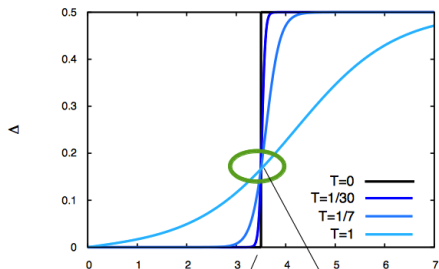
$$\Delta_{att}^{hf}(\eta) = \frac{1}{2} \frac{\sinh(\beta\eta)}{\cosh(\beta\eta) + e^{-\beta\frac{|U|}{2}}}$$



$n_s = 5$

Repulsive $U > 0$

$$\Delta_{rep}^{hf}(\eta) = \frac{1}{2} \frac{\sinh(\beta\eta)}{\cosh(\beta\eta) + e^{\beta\frac{U}{2}}}$$



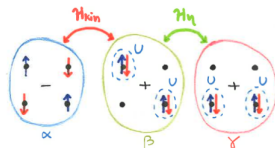
$|U| = 7D$

$$\eta = \frac{U}{2} \quad |\uparrow\rangle \rightarrow \frac{|\uparrow\downarrow\rangle - |0\rangle}{\sqrt{2}}$$

Why is the second derivative sensitive to preformed pairs?

Two-sites model: ground state

$$H = H_{\text{kin}} + H_U + H_\eta$$



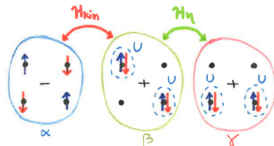
Ground State Crossover

$$|\text{GS}\rangle = \underbrace{\alpha \left(\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \right)}_{\text{localized momenta}} + \underbrace{\beta \left(\frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \right) + \gamma \left(\frac{|0, 0\rangle + |\uparrow\downarrow, \uparrow\downarrow\rangle}{\sqrt{2}} \right)}_{\text{localized preformed pairs}}$$

Why is the second derivative sensitive to preformed pairs?

Two-sites model: ground state

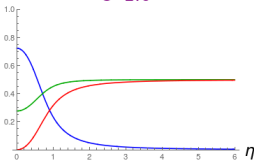
$$H = H_{\text{kin}} + H_U + H_\eta$$



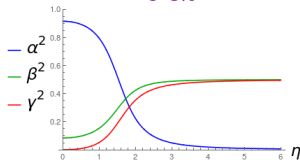
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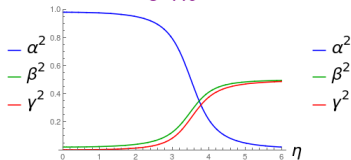
U=1.0



U=3.0



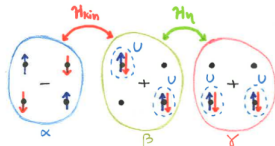
U=7.0



Why is the second derivative sensitive to preformed pairs?

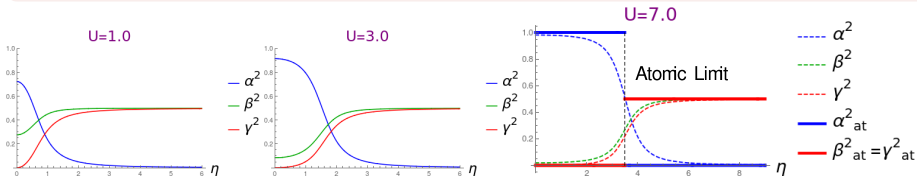
Two-sites model: ground state

$$H = H_{\text{kin}} + H_U + H_\eta$$



Ground State Crossover

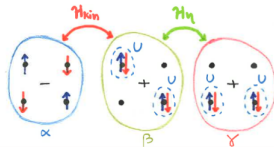
$$|\text{GS}\rangle = \underbrace{\alpha \left(\frac{|\uparrow\downarrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} \right)}_{\text{localized momenta}} + \underbrace{\beta \left(\frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \right) + \gamma \left(\frac{|0, 0\rangle + |\uparrow\downarrow, \uparrow\downarrow\rangle}{\sqrt{2}} \right)}_{\text{localized preformed pairs}}$$



Why is the second derivative sensitive to preformed pairs?

Two-sites model: ground state

$$H = H_{\text{kin}} + H_U + H_\eta$$



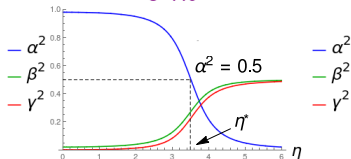
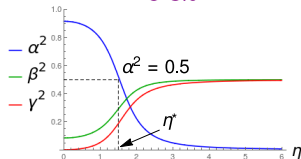
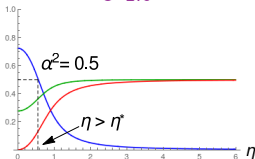
Ground State Crossover

$$|\text{GS}\rangle = \underbrace{\alpha \left(\frac{|\uparrow\downarrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} \right)}_{\text{localized momenta}} + \underbrace{\beta \left(\frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \right) + \gamma \left(\frac{|0, 0\rangle + |\uparrow\downarrow, \uparrow\downarrow\rangle}{\sqrt{2}} \right)}_{\text{localized preformed pairs}}$$

U=1.0

U=3.0

U=7.0



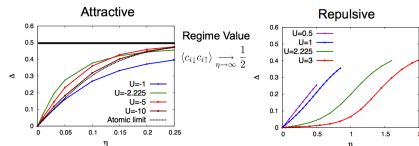
Physical interpretation of $\eta^* \Rightarrow$ change of the main character of the GS



Interpretation

Highlights of the results

- **Suppression** of the **linear response** for $U > 0$
- **Positive second derivative** \nRightarrow **absence** of preformed pairs



Physical interpretation

Linear response \rightarrow Fluctuation-Dissipation theorem

Second derivative $\frac{\partial^2 \Delta(\eta)}{\partial \eta^2} \rightarrow$ direct **physical meaning?**

Main **GS character** crossover: **AFM** \rightarrow **SC**



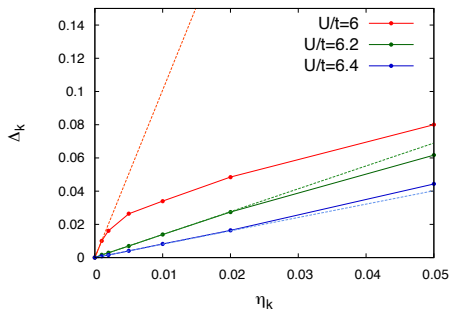
Testing preformed pairs in pseudogap region

E. Gull and A. J. Millis *Phys. Rev. B* **86** (2012)

DCA calculations in a repulsive Hubbard model under a *d-wave* external pairing field

- ⇒ Inclusion of short range spatial correlations
- ⇒ Explicit d-wave superconducting symmetry breaking

$$\Delta_{\mathbf{k}}(\eta_{\mathbf{k}})|_{\mathbf{k}=(0,\pi)}$$



Abrupt response suppression for $U > 5.9t$

Solid interpretation of the results
beyond the linear response

$$\left. \frac{\partial^2 \Delta}{\partial \eta^2} \right|_{U=6.4t} > 0$$

No preformed pairs

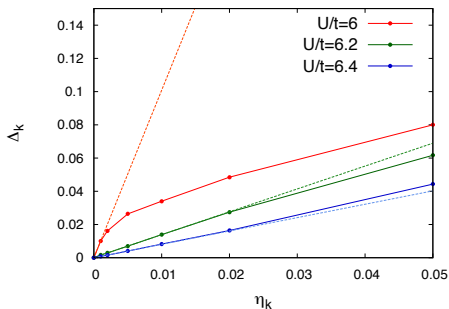
Testing preformed pairs in pseudogap region

E. Gull and A. J. Millis *Phys. Rev. B* **86** (2012)

DCA calculations in a repulsive Hubbard model under a ***d*-wave** external pairing field

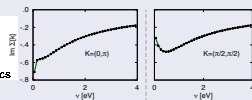
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$$\Delta_{\mathbf{k}}(\eta_{\mathbf{k}})|_{\mathbf{k}=(0,\pi)}$$

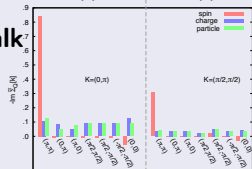


See other works:

- J. Merino and O. Gunnarsson *PRB* (2014)
- O. Gunnarsson, T. Schäfer, J. P. LeBlanc, E. Gull, J. Merino, G. Sangiovanni, G. Rohringer, and A. Toschi *PRL* (2015)



See next talk



Conclusions and Outlook

Conclusions and Outlook

Results

DMFT studies under a pairing forcing field η : **Attractive** vs **Repulsive** Hubbard model

- **Second order** response
 - $U < 0 \Rightarrow \frac{\partial^2 \Delta(\eta)}{\partial \eta^2} < 0$ (preformed pairs)
 - $U > 0 \Rightarrow \frac{\partial^2 \Delta(\eta)}{\partial \eta^2} > 0$ for $\eta \in [0, \eta^*)$ (no preformed pairs)
- Physical understanding: **two-sites model**

$\Delta(\eta)$ inflection point \Leftrightarrow GS main character change

- Improving interpretation of DCA results

$$\frac{\partial^2 \Delta_{\mathbf{k}}}{\partial \eta_{\mathbf{k}}^2} \Big|_{\mathbf{k}=(0,\pi)} > 0 \Rightarrow \text{No preformed pairs}$$

Outlook

- Probe different ordered phases
- Detect localized magnetic moments with a physical field
- Connection with **out-of-equilibrium** experiments

Thank you for the attention!