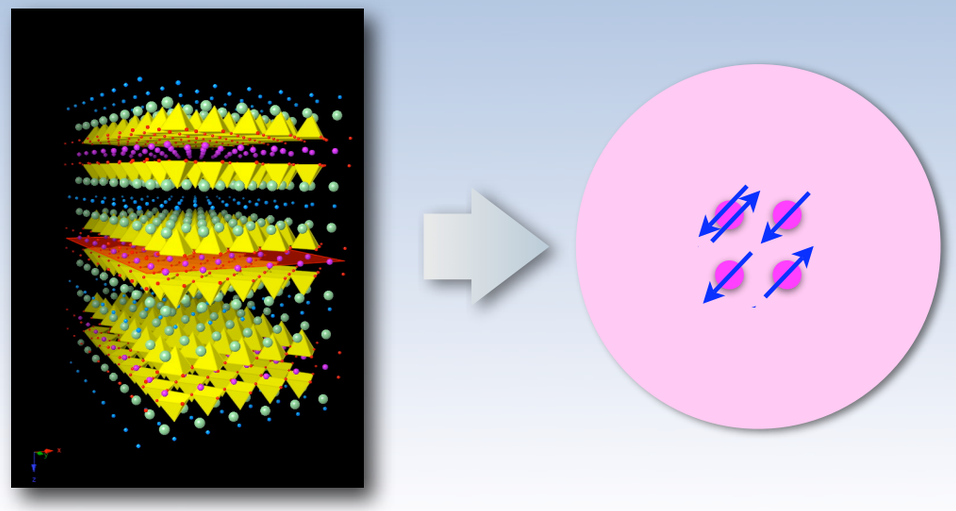
Dynamic cluster simulations of high-temperature superconductors:
Scientific Impacts and Opportunities

T.A. Maier, ***Oak Ridge National Laboratory***

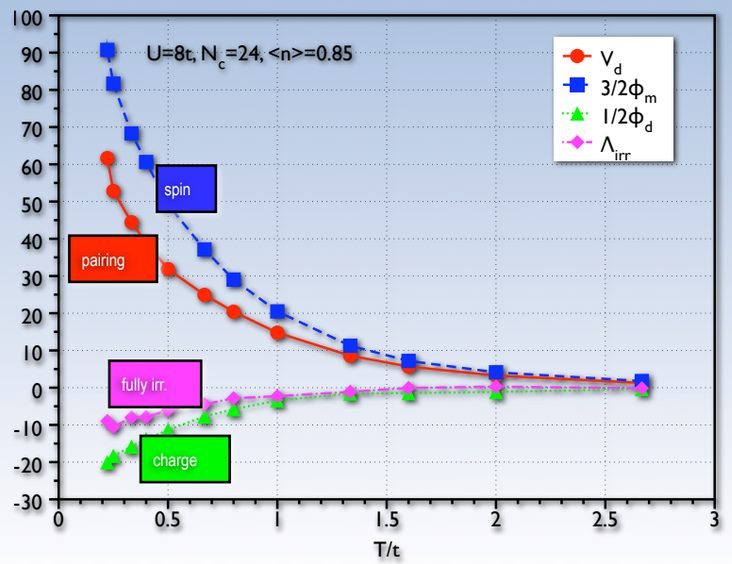
Oak Ridge National Lab	University of Cincinnati	University of California
G. Alvarez P. Kent T. A. Maier T.C. Schulthess D. Abernathy P. Dai H. Mook	M. Jarrell	D. Scalapino

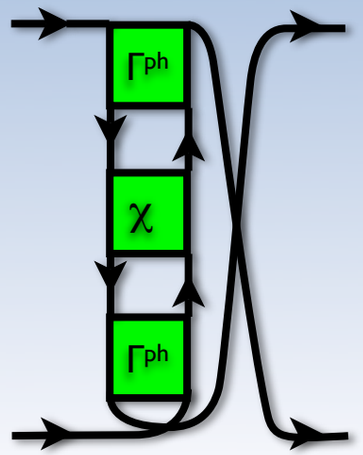
Outline

Dynamic cluster simulations of cuprates

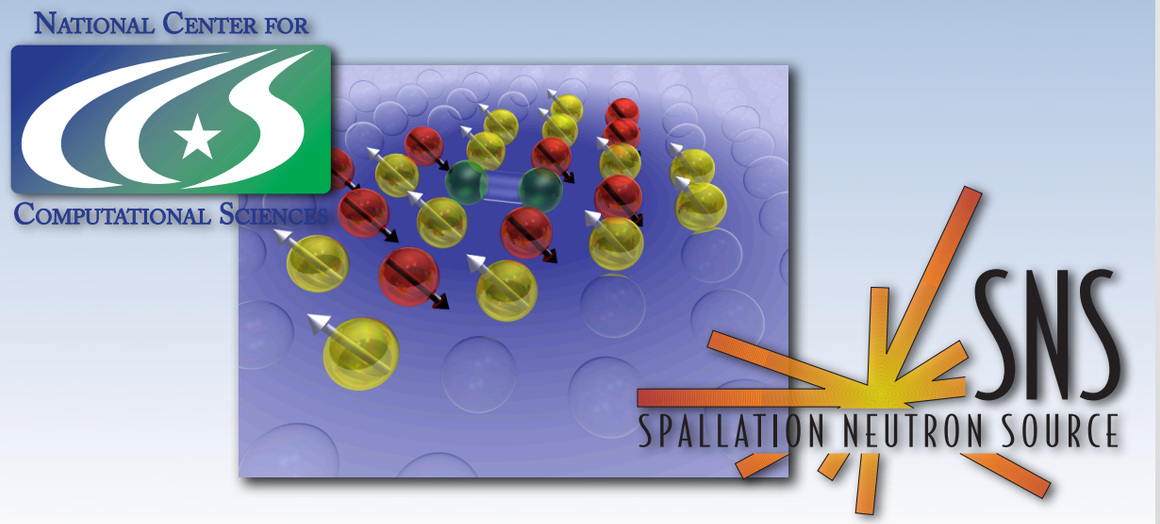


New scientific insights

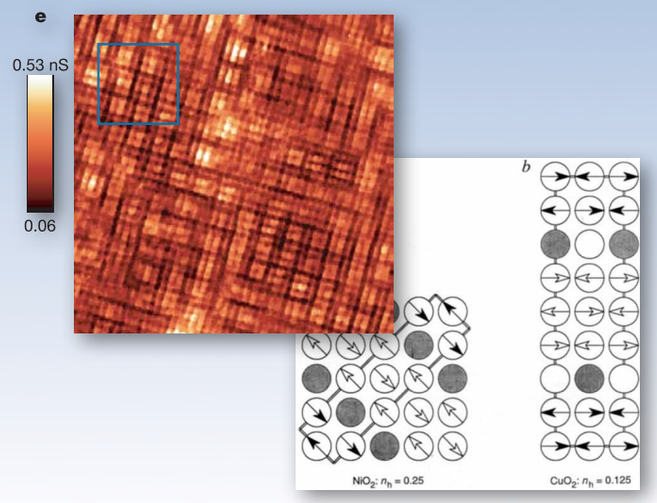




Validation with neutron scattering

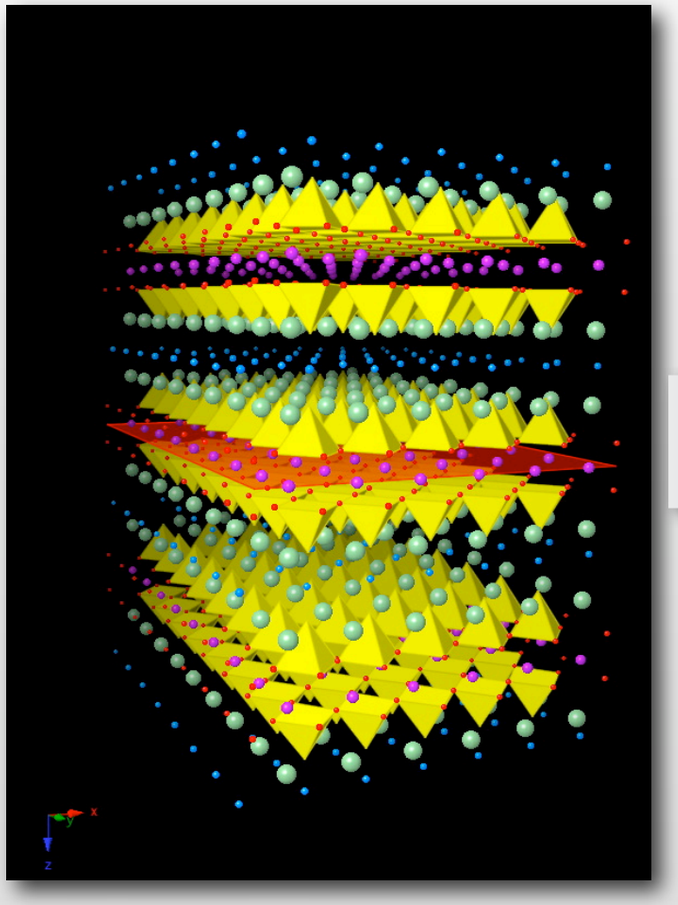


Spatial inhomogeneities in cuprates

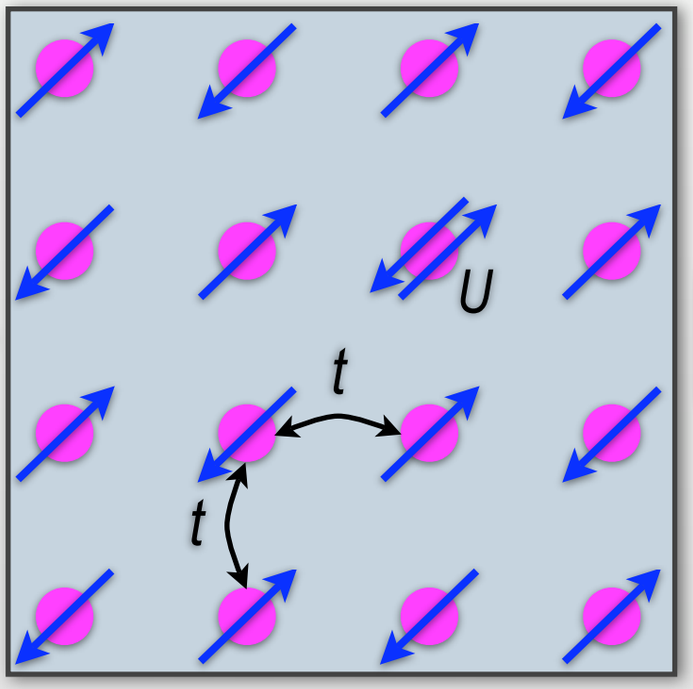


Quantum Cluster methods reduce complexity

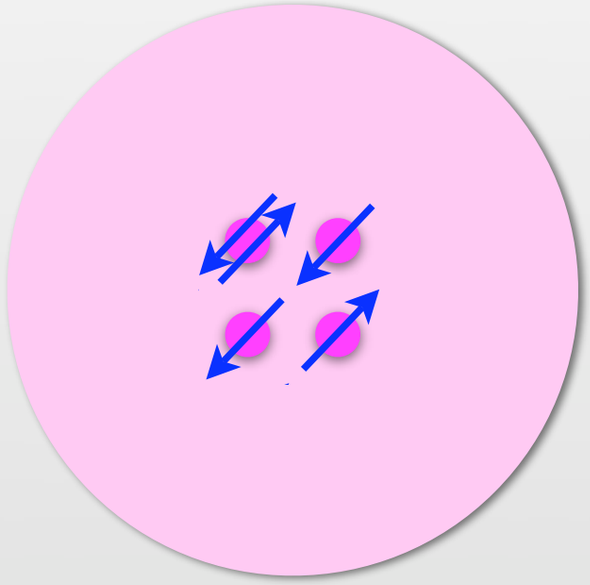
HTSC: 10^{23}
interacting electrons



2D Hubbard model
for CuO planes



Dynamic cluster
approximation: Map
Hubbard model onto
embedded cluster



> Correlations within cluster treated explicitly
> Correlations beyond cluster treated in mean-field
> DCA: Cluster in k-space Hettler *et al.*, PRB '98

Quantum cluster theories: T.A. Maier *et al.*, RMP '05

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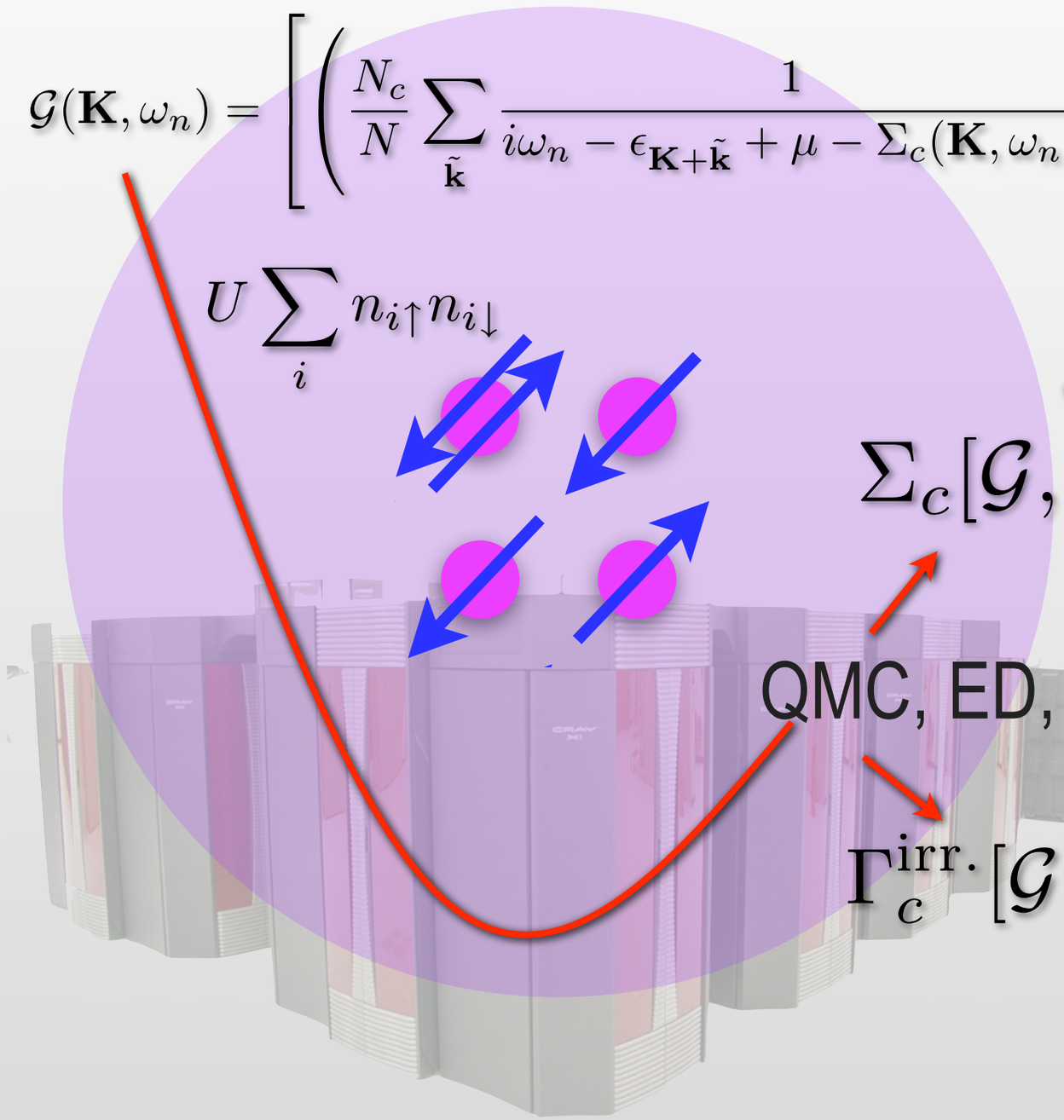
DCA: Self-consistent Algorithm

$$\mathcal{G}(\mathbf{K},\omega_n) = \left[\left(\frac{N_c}{N}\sum_{\tilde{\mathbf{k}}}\frac{1}{i\omega_n - \epsilon_{\mathbf{K}+\tilde{\mathbf{k}}} + \mu - \Sigma_c(\mathbf{K},\omega_n)}\right)^{-1} + \Sigma_c(\mathbf{K},\omega_n)\right]^{-1}$$



$$\Sigma_c[\mathcal{G},U]$$

Single-particle properties:
> Fermi surface
> ARPES
> QP weight, ...

QMC, ED, NCA, ...

$$\Gamma_c^{\text{irr.}}[\mathcal{G},U]$$

Two-particle properties:
> S(Q,ω)
> Phase transitions, ...

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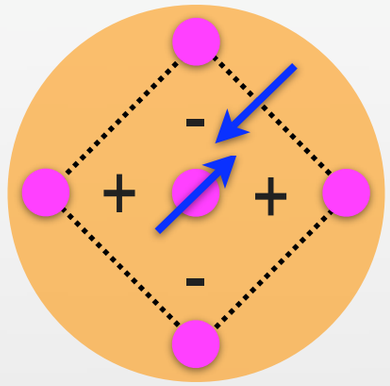
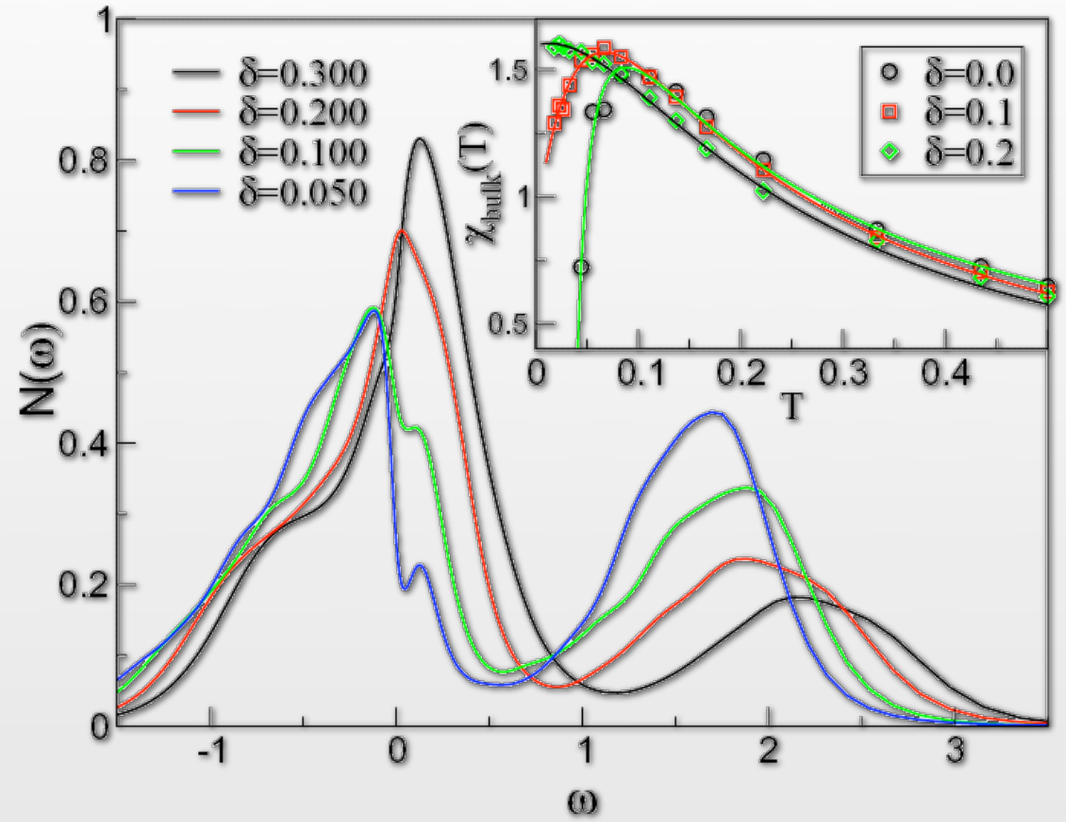
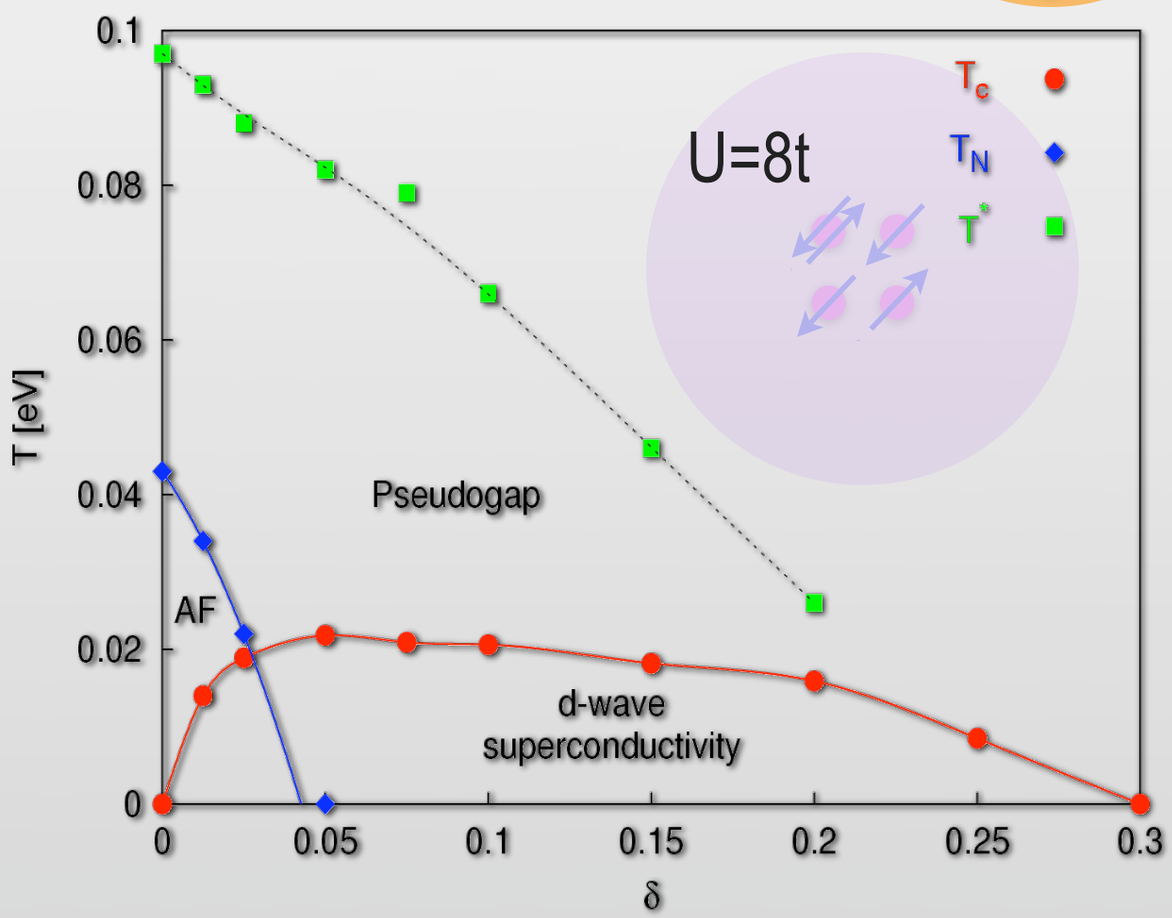
DCA small cluster (4-site) phase diagram

4-site plaquette is smallest cluster that can describe d-wave SC







4-site phase diagram:

- ✓ AF
- ✓ D-wave SC
- ✓ Pseudogap

(M. Jarrell et al., EPL '01; CDMFT: Kyung *et al.*, PRB '06, Kancharla *et al.*, preprint '06; CPT: Sénéchal *et al.*, PRL, '04, '05; Aichhorn *et al.*, PRB '06)

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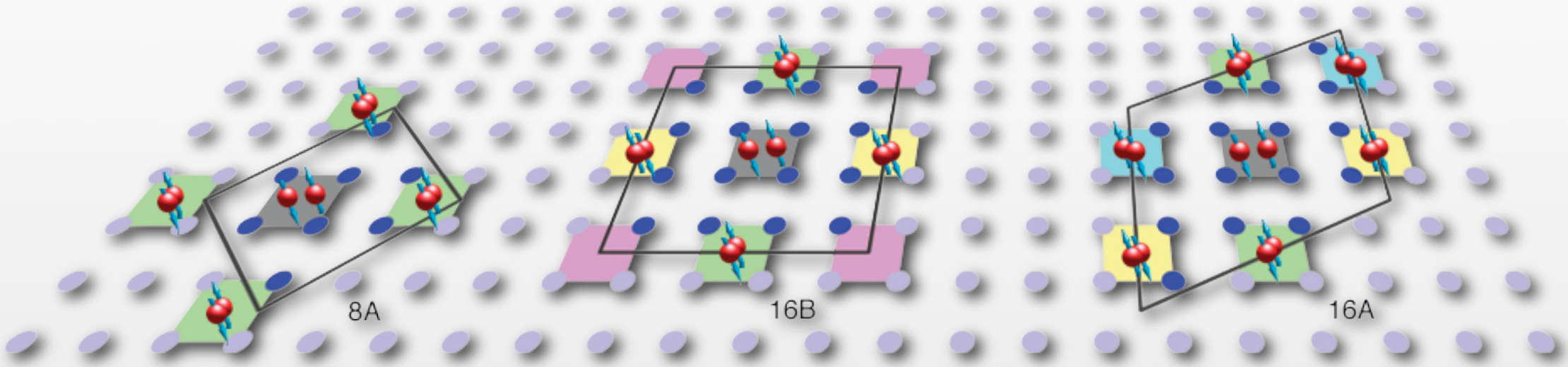
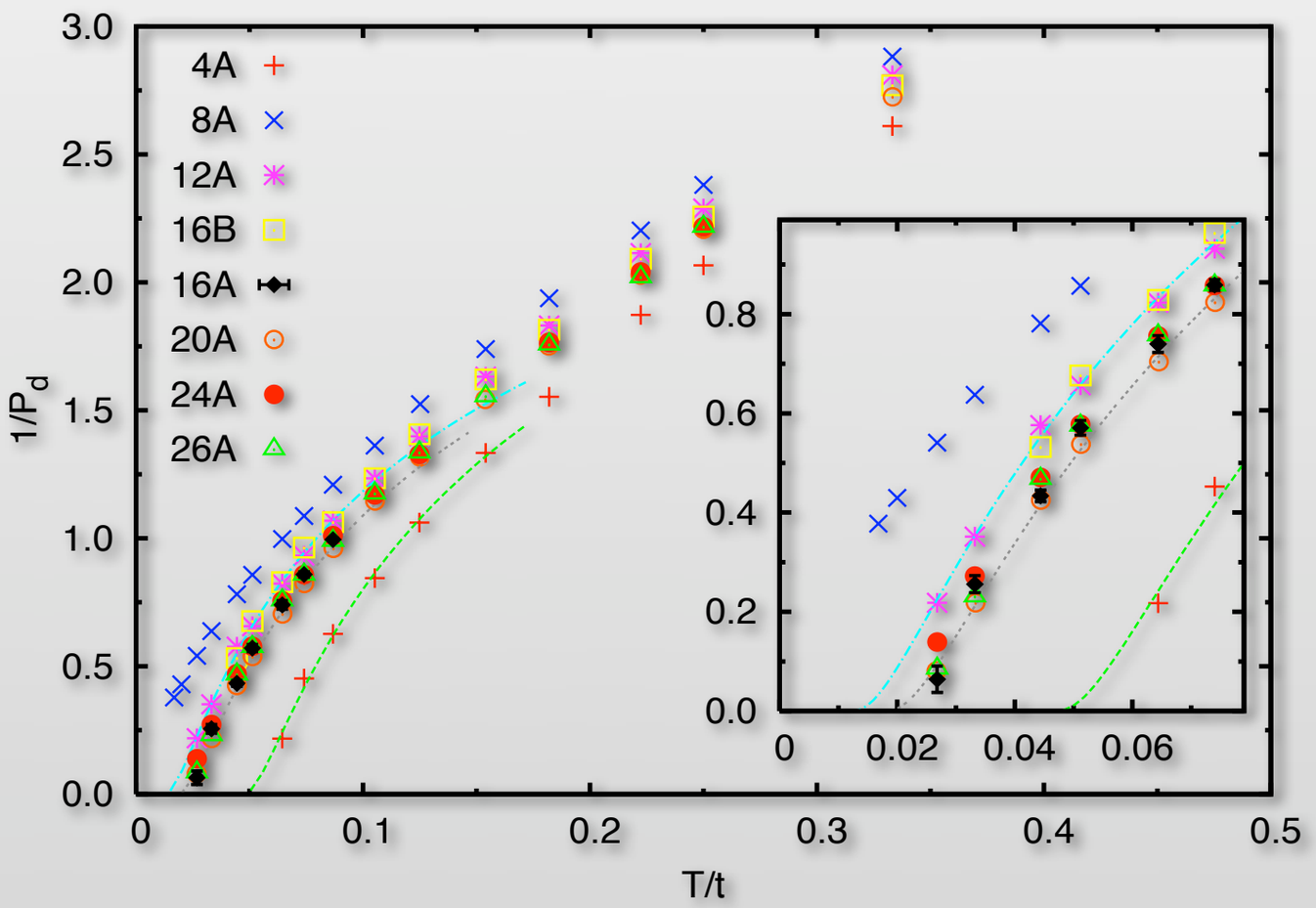
Superconductivity as a consequence of electronic correlations





N_c	Z_d	T_c
4A	0	0.056
8A	1	-0.006
12A	2	0.016
16B	2	0.015
16A	3	0.025
20A	4	0.022
24A	4	0.020
26A	4	0.023

(TAM *et al.*, PRL '05)

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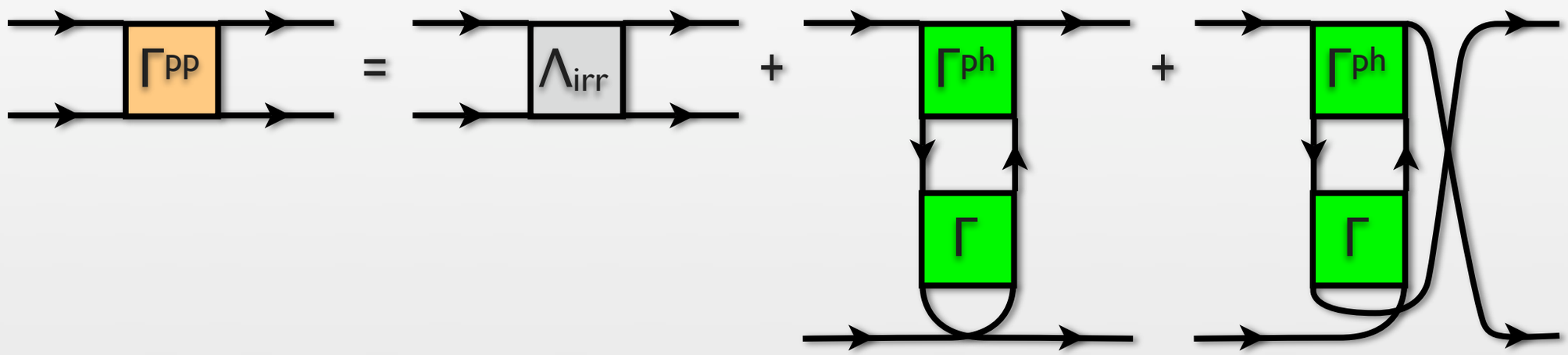
Pairing interaction from an orthogonal perspective

Pairing Interaction



Mechanism

(Pfitzner, Wölfle, PRB '89; Esirgen, Bickers, PRB '98)

Calulate with DCA/QMC

Maier *et al.*, PRL '06

$$\Gamma^{pp}(K|K') = \Lambda_{irr}(K|K') + \frac{1}{2}\Phi_d(K|K') + \frac{3}{2}\Phi_m(K|K')$$

Pairing interaction — fully irreducible — Charge — Spin

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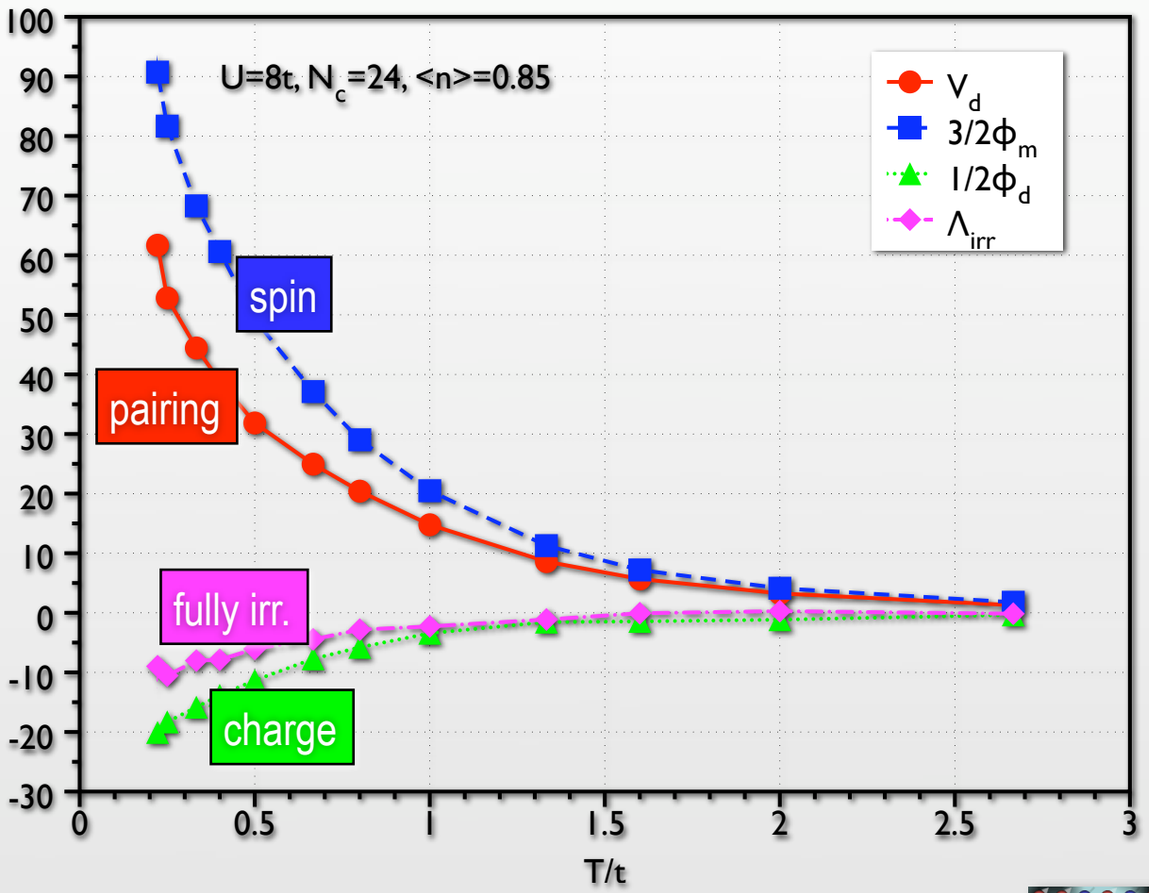
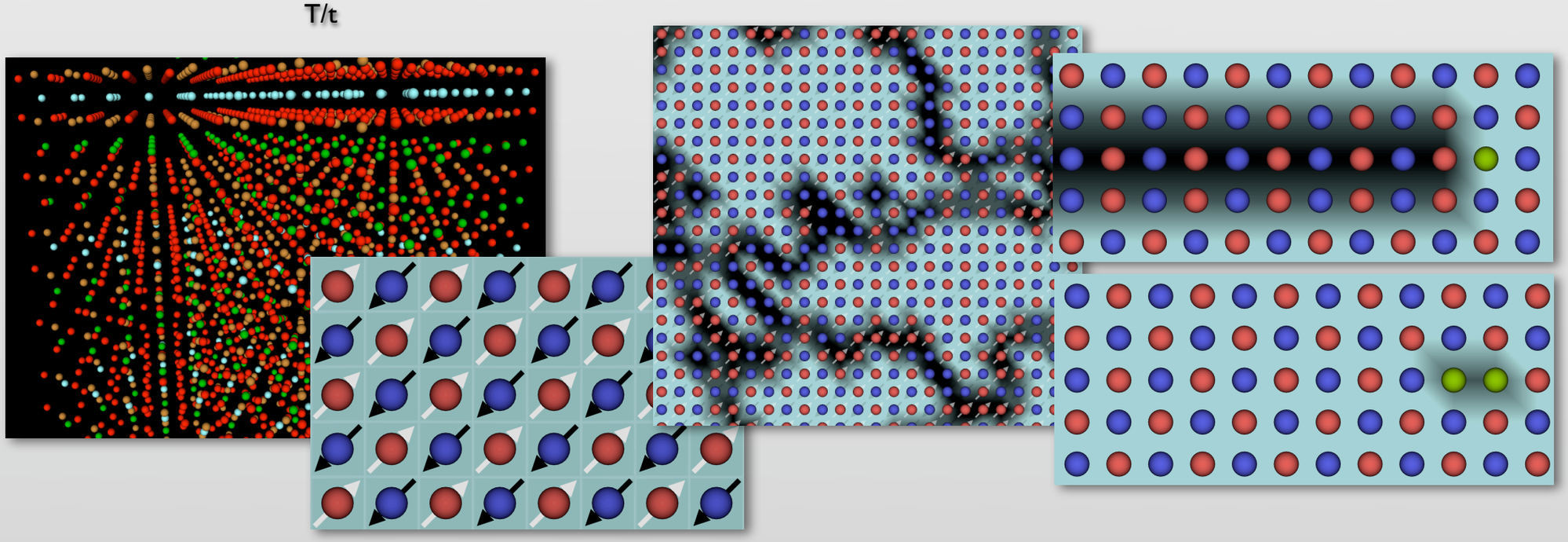
Magnetic origin of pairing interaction



- Attractive pairing interaction between nearest neighbor singlets
- Dynamics associated with antiferromagnetic spin fluctuation spectrum
- Pairing interaction mediated by antiferromagnetic spin fluctuations

Maier *et al.*, PRL '06, PRB '06, PRB '07



Simple picture:
Superconductivity from electronic correlations

- Physics dominated by Coulomb energy, kinetic energy is frustrated

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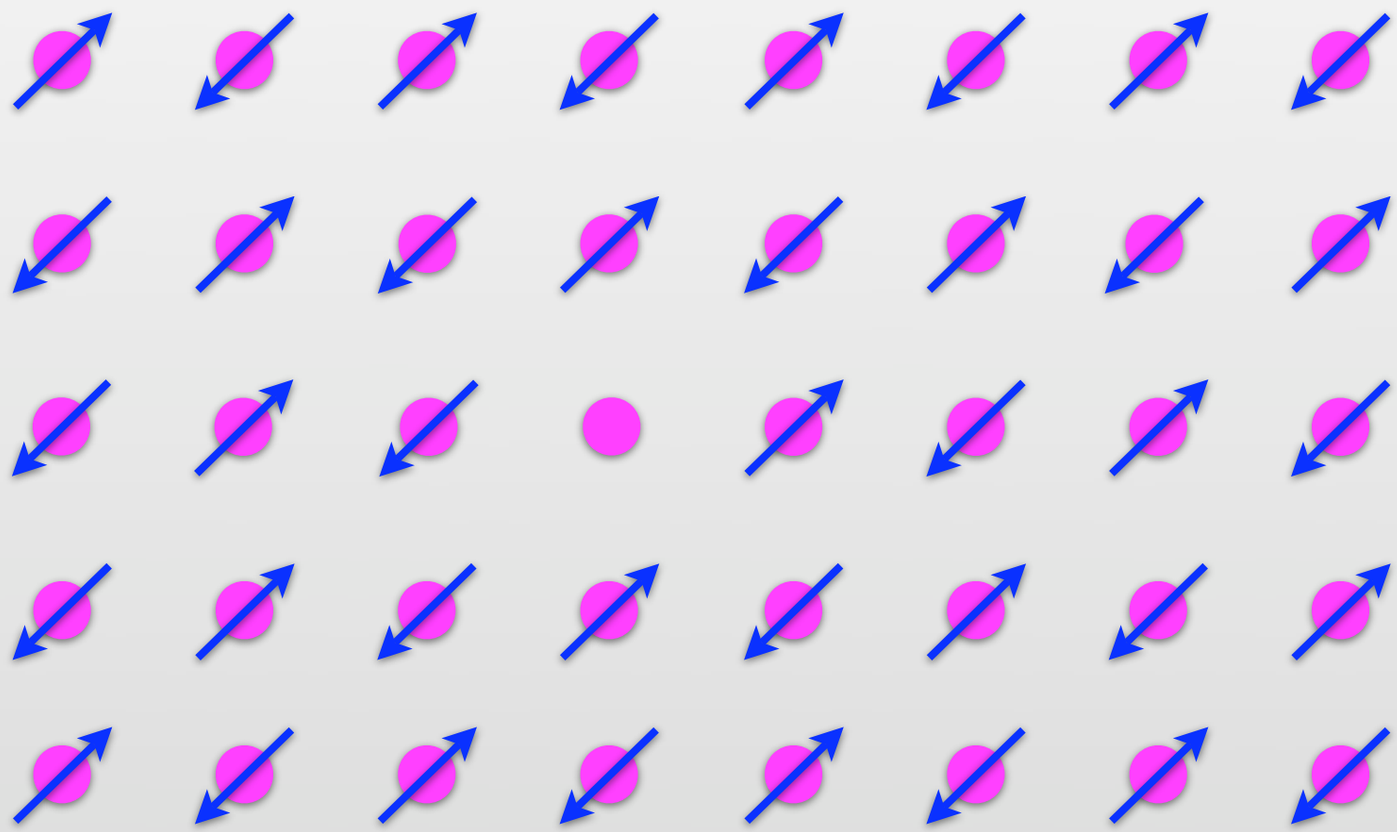

Simple picture: Superconductivity from electronic correlations

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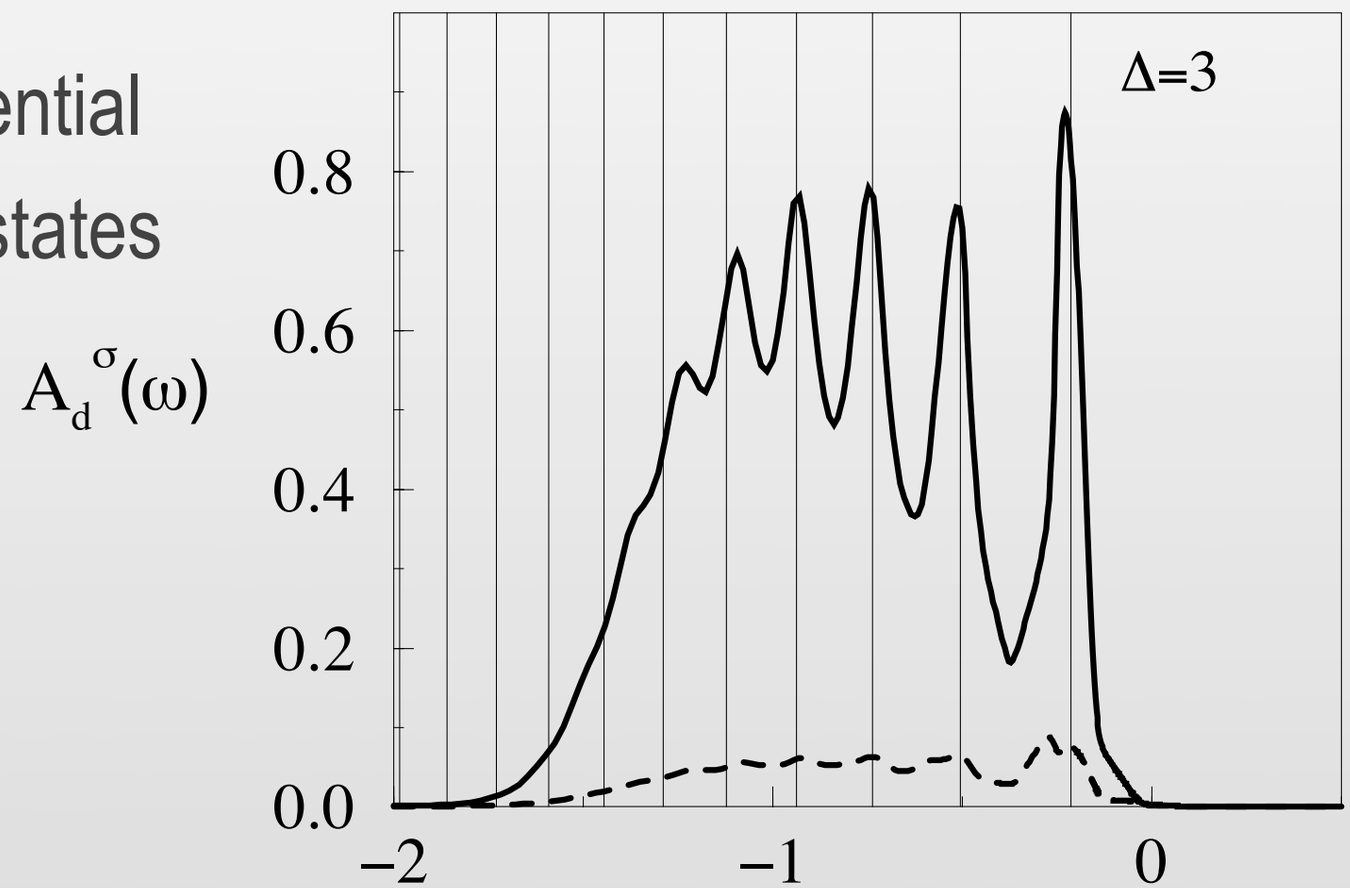
> Confining potential

> D=∞: Bound states



TAM *et al.*, Eur. Phys. J. B, '99

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Pairing: a way to relieve kinetic frustration

- Paired hole restores antiferromagnetic background
  (Brinkman, Rice PRB '70; Hirsch, PRL '87; Bonca *et al.*, PRB '89; Dagotto *et al*., PRB '90)

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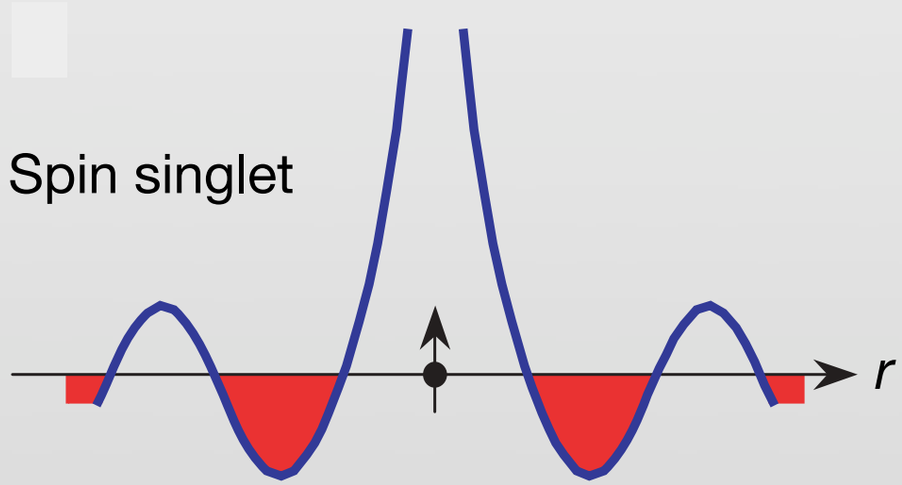
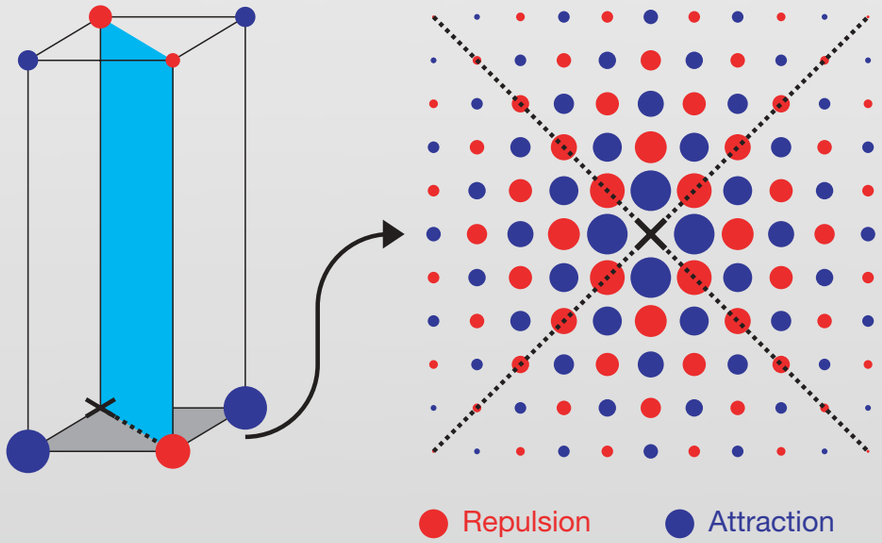
Magnetically mediated superconductivity: Intuitive picture

Review: Monthoux *et al.*, Nature '07

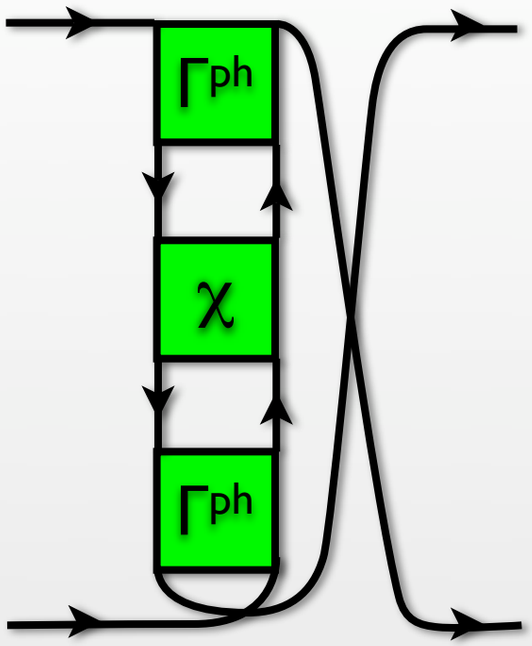
- Spin s' generates magnetic interaction field of strength $\bar{U}s'$
- Field induces magnetic moment given by $m(r,t)=\bar{U}s'\chi(r,t)$
- Spin s at position r feels effective moment as $\bar{U}m(r,t)$
- Effective interaction takes the form $-\bar{U}^2\, s.s'\chi(r,t)$



Border of antiferromagnetism



Spin-susceptibility representation enables neutron scattering validation



Test simple spin-susceptibility representation of pairing interaction and calculate T_c in Hubbard model

$$\Gamma^{pp}(K,K') \overset{?}{\approx} \frac{3}{2}\bar{U}^2\chi(K-K')$$

electron filling	<n>	0.95	0.90	0.85
"exact" QMC	T_{c0}	0.080	0.074	0.067
$\bar{U}$ fitted from Γ^{pp}	$T_{c0}^{(1)}$	0.100 (25%)	0.087 (18%)	0.074 (10%)
$\bar{U}$ from single-particle spectrum	$T_{c0}^{(2)}$	0.108 (35%)	0.084 (14%)	0.064 (4%)
$\bar{U}$, G fitted from single-particle spectrum	$T_{c0}^{(3)}$	0.105 (31%)	0.081 (9%)	0.058 (13%)

Maier *et al.*, PRB '07

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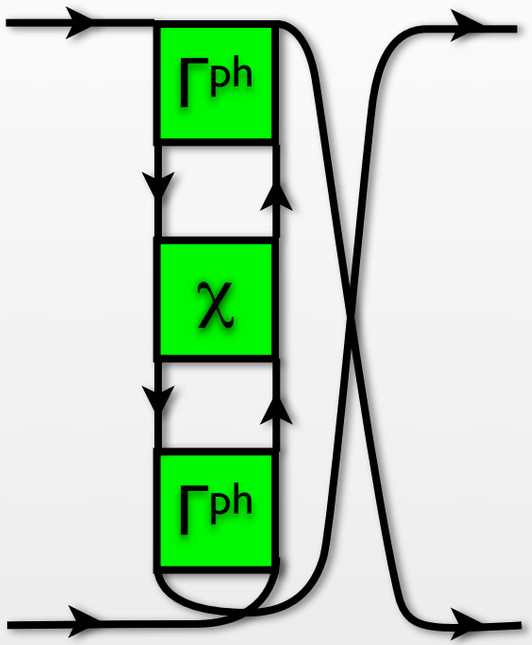

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$$\Gamma^{pp}(K,K') \overset{?}{\approx} \frac{3}{2}\bar{U}^2\chi(K-K')$$
$$+\bar{J}(\cos K_x - \cos K_y)(\cos K'_x - \cos K'_y)$$

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Maier *et al.*, PRB '07

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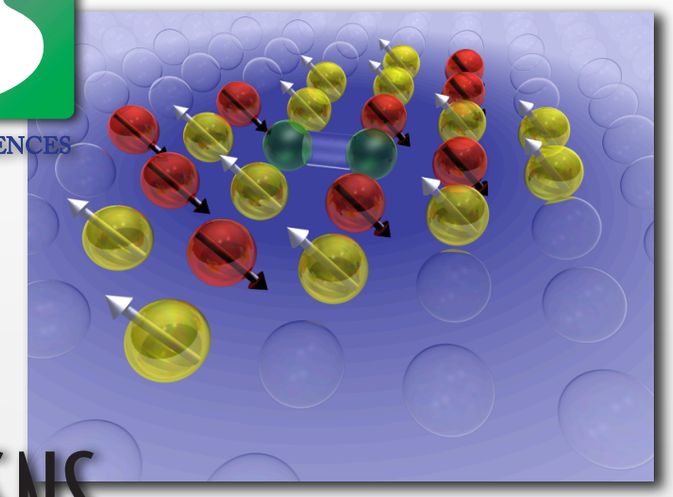
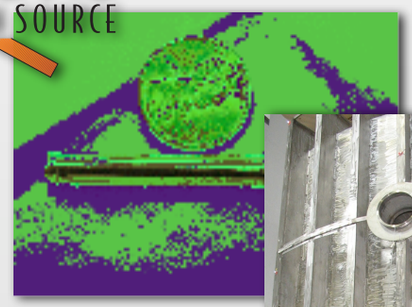
High-impact science?

- Computational predictions
  - If spin fluctuations are responsible for pairing, we can calculate the superconducting transition temperature T_c from the spin susceptibility
  - The spin susceptibility can be measured in neutron scattering experiments
- Experiments to validate predictions
  - Neutron scattering studies on high-T_c cuprates to measure the dynamic spin susceptibility
  - Use neutron data as input to calculate T_c based on Hubbard model simulations
  - Compare estimate of T_c with actual T_c





Almost certainly a success

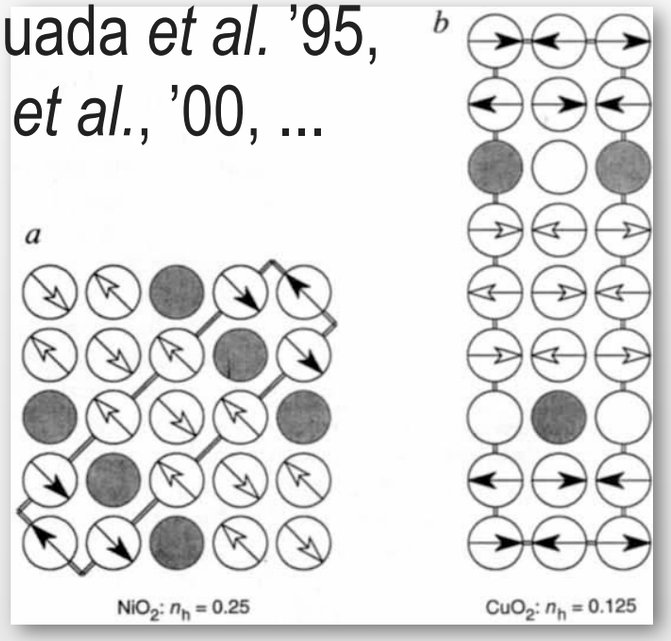
> *Positive outcome* → *Solution of one of the most important problems in condensed matter science*

> *Negative outcome* → *Hubbard model - commonly accepted to describe the cuprates - does not have the right stuff*

What is missing in this picture?
Spatial inhomogeneities in cuprates

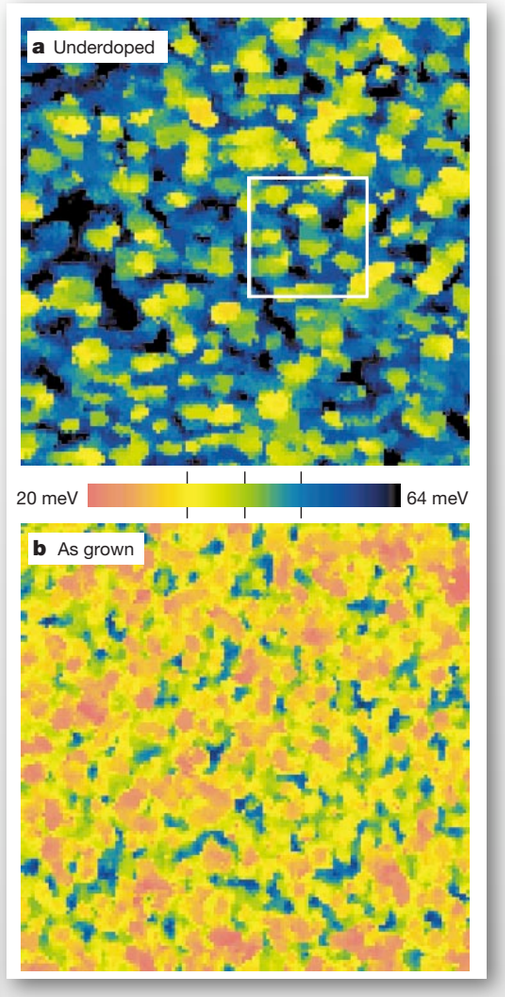
Stripes in neutron scattering:

Tranquada *et al.* '95,
Mook *et al.*, '00, ...



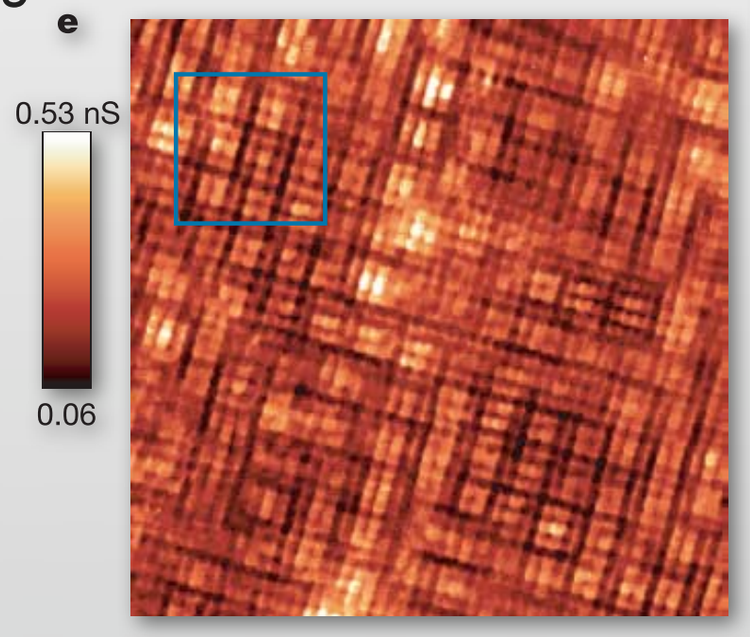
Random SC gap modulations in STM (BSCCO):

Lang *et al.* '02



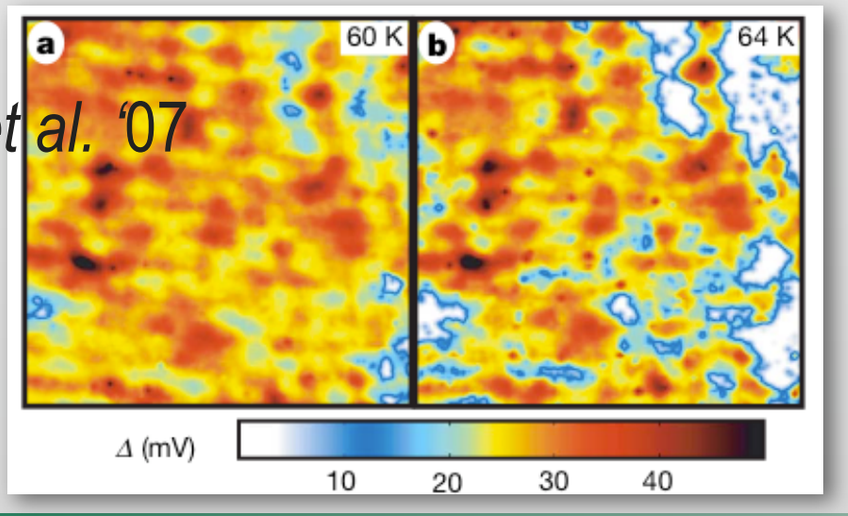
Charge ordered "checkerboard" state (Na doped cuprates):

Hanaguri *et al.* '04



Random gap modulations above T_c (BSCCO):

Gomes *et al.* '07



Stripes: another way to relieve kinetic energy frustration

- Phase separation into hole rich and hole poor regions was predicted by theory (Gor'kov '87, Zaanen *et al.*, '89, Emory *et al.*, '90, White, Scalapino, '98)

- Inhomogeneities not included in present models

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The role of inhomogeneities in cuprates: An open problem

- Is superconductivity mediated by inhomogeneities?
- Do they enhance or suppress pairing?
- Is there an "optimal" inhomogeneity that maximizes T_c?

  Emory, Kivelson *et al.*, many papers

- Theoretical studies are difficult
  - Strong electron correlations + inhomogeneities
  - Present models are too simple to describe the real situation in the cuprates

- Need to solve appropriate models
- Opportunity for high-end computing

Research plan: Inhomogeneities in the Hubbard model

- Study how inhomogeneities affect superconductivity in the 2D Hubbard model
  - Random local Coulomb repulsions $U(R_i)$
  - Periodic modulations of Coulomb repulsion
  - Varied doping in multi-layer systems
- Questions to study in the near term
  - Do inhomogeneities increase or decrease the transition temperature?
  - How do they affect the pairing interaction?
  - What is their effect on the electronic spectrum?
- Questions to study in the long term
  - Is there an optimal inhomogeneity that maximizes the transition temperature?
  - Is there an experimental realization of optimal inhomogeneous system?
- Relevance to experimental program
  - LSCO films and super-lattices with varied doping in growth direction can be grown at CNMS
  - Systems can be characterized with neutron scattering

Scientific and technological impact

- Scientific impact:
  - Understand the role of inhomogeneities in the cuprates, their effect on superconductivity including the transition temperature as well as the pairing interaction
  - Important step towards solving the high-Tc puzzle
- Potential technological impact:
  - Predict optimal in-plane inhomogeneity to artificially structure cuprate based materials with higher transition temperatures
  - Predict optimal layer-dependent doping for multi-layer systems that maximizes transition temperature

Research plan: Material specific calculations

- Link models to real materials
  - Generate material specific models with DFT-based ab-inito calculations
  - Understand the large differences in critical temperatures between different cuprates

→ T.C. Schulthess

Summary

- Dynamic cluster simulations of 2D Hubbard model of high-temperature superconducting cuprates
- Superconductivity as a result of strong electronic correlations
- Pairing mediated by spin-fluctuations
- Missing:
  - Experimental validation
  - Inclusion of charge and spin inhomogeneities

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Research Plan

How does inhomogeneity affect superconductivity?

Simulate Hubbard model with random disorder in inter-action strength

12 month

Is there an optimal inhomogeneity?

Simulate Hubbard model with periodically modulated disorder & varied doping in multilayers

18 month

Is high-temperature superconductivity mediated by spin fluctuations?

Perform & analyze neutron scattering experiments on cuprates to validate simulations

2 years

Why is there a factor 5 difference in T_c between different cuprates

Generate & simulate material specific multi-band models of cuprates

5 years