

# The superconducting phase diagram in a model for tetragonal and cubic systems with strong antiferromagnetic correlations

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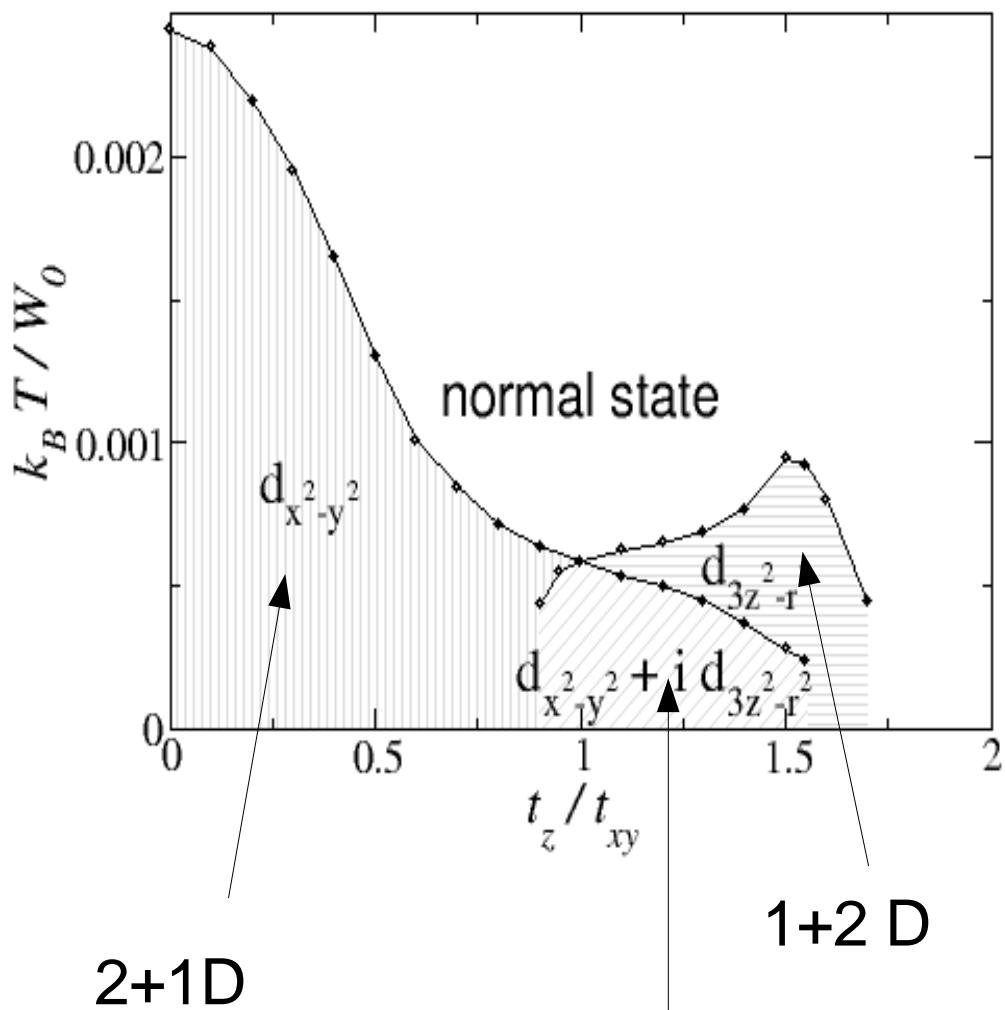
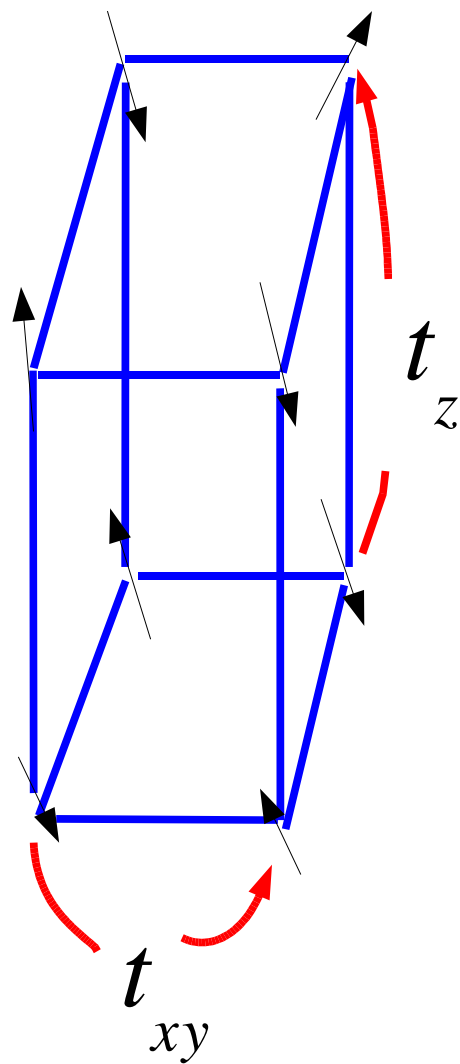
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Thomas Maier (ORNL)  
UNI Graduate College

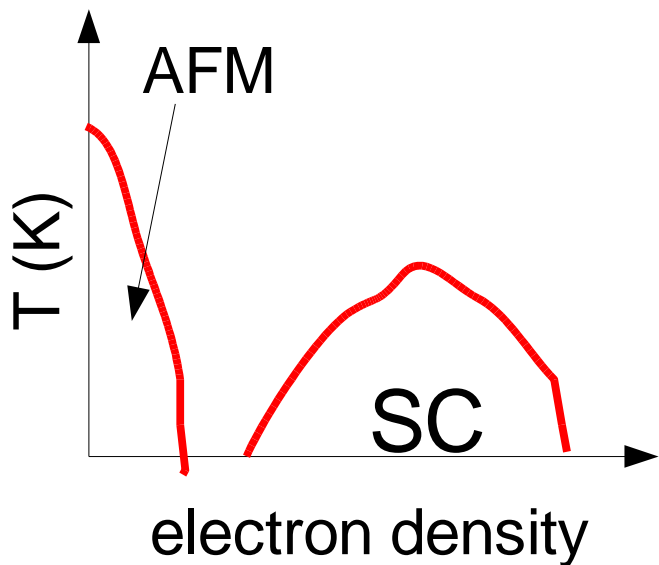
## Outline:

Pair wavefunction in superconductors  
Antiferromagnetism and d-wave pairing  
Lattice symmetry and d-wave pairing  
Method and model  
Results

# Upshot: possible phase diagram for AFM-mediated superconductivity



3D: T-breaking



# Pair wavefunction in superconductors

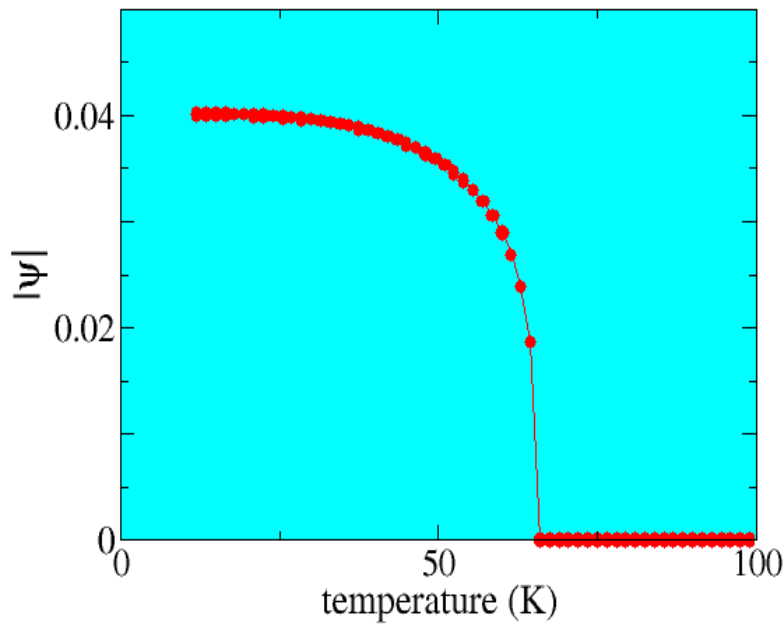
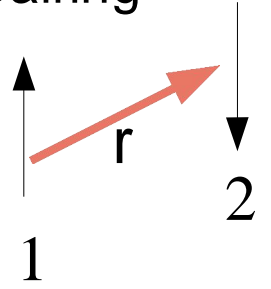
- Enhanced electron pair correlations, i.e. electron pairing
- Pairs are described by a two-body wavefunction:

$$\Psi(r_1, r_2) = \psi(r_{cm}) \phi(r) \chi(\sigma_1, \sigma_2)$$

- Wavefunction is antisymmetric under exchange

$$\phi(-r) \chi(\sigma_2, \sigma_1) = -\phi(r) \chi(\sigma_1, \sigma_2)$$

- $|\psi|=0$  in the normal state,  $|\psi| > 0$  for a superconductor



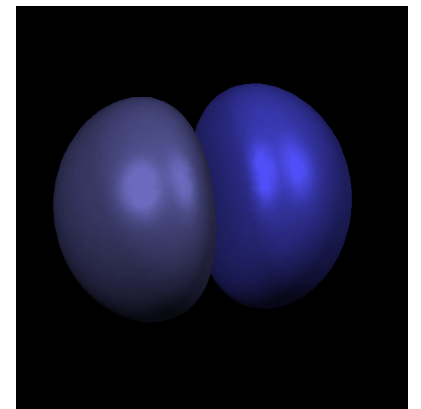
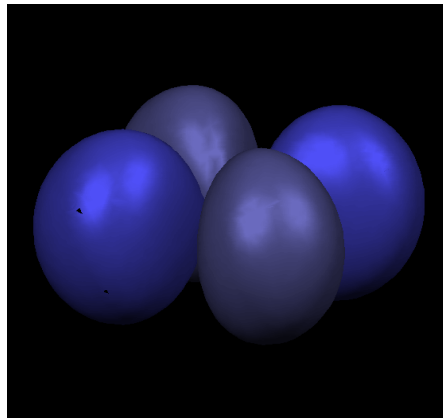
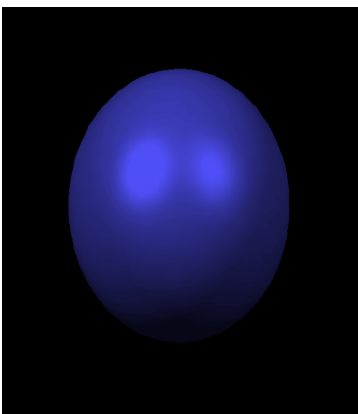
$$\chi(\sigma_1, \sigma_2) = | \uparrow \uparrow \rangle$$

$$| \uparrow \downarrow \rangle + | \downarrow \uparrow \rangle$$

$$| \downarrow \downarrow \rangle$$

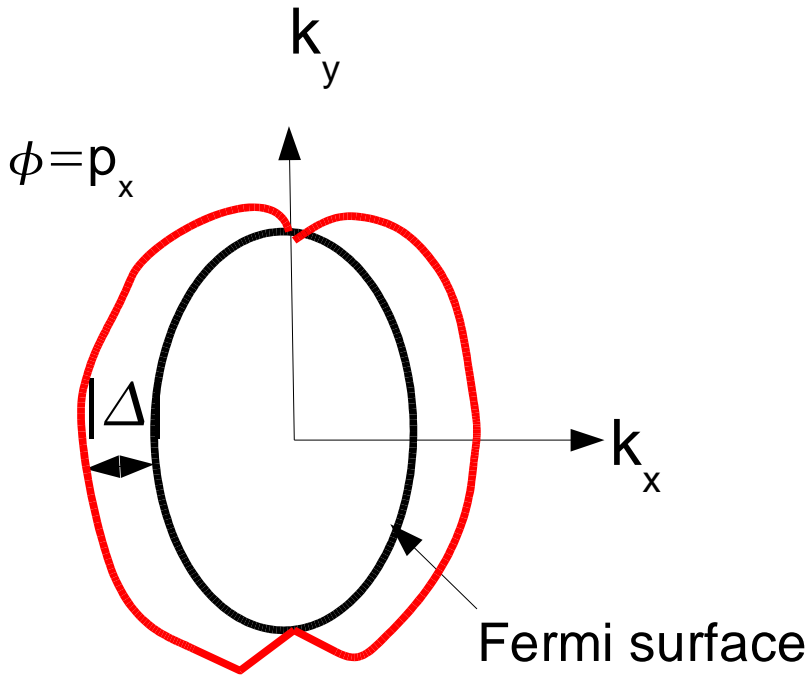
$$\chi(\sigma_1, \sigma_2) = | \uparrow \downarrow \rangle - | \downarrow \uparrow \rangle$$

$\phi(r)$



# Pair wavefunction in superconductors

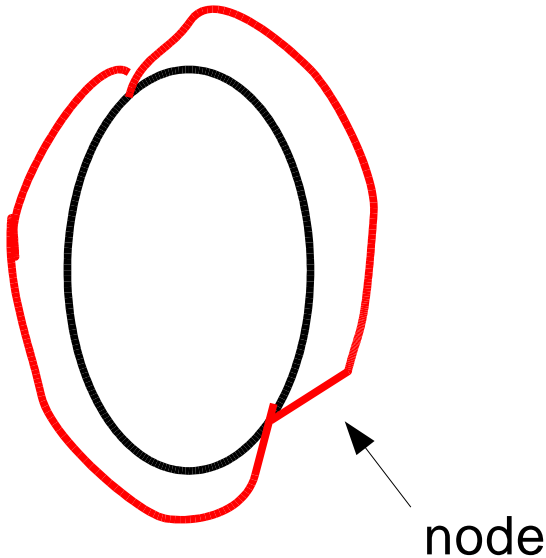
- Superconducting gap:  $\Delta(k) \approx \psi \int dr \exp(i k \cdot r) \phi(r)$



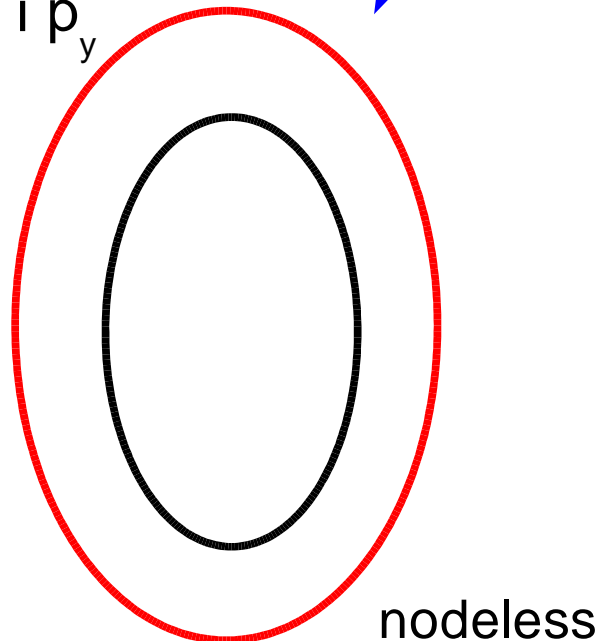
- s-like  $\phi$ 's are non-degenerate
- p- and d-like  $\phi$ 's can be degenerate

T-breaking,  
energetically  
favored for weak-  
coupling

$\phi = p_x \pm p_y$



$\phi = p_x \pm i p_y$



# Antiferromagnetism and $\phi=d$ pairing

- Cuprates (2D): strong AFM correlations,  
d-wave pairing

- (3D)  $\text{CeIn}_3$ , (2D)  $\text{CeRhIn}_5$ , ...

- (2D) Monthoux, Balatsky  
and Pines (1991, 1992)

\* inputs:

electronic properties  
electron-AFM coupling  
AFM correlations

\* output:

$\phi = d (x^2 - y^2)$

- (2D) Pao and Bickers,  
Monthoux and Scalapino (1993)

\* microscopic: Hubbard model + perturbation theory

\*  $\phi = d (x^2 - y^2)$  pair wavefunction

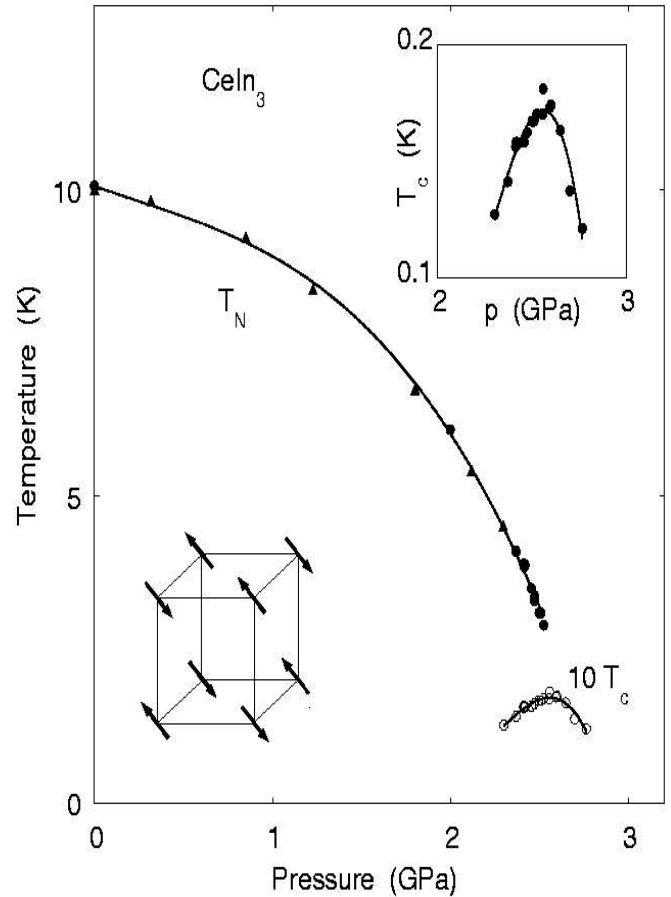
- (3D) Monthoux and Lonzarich (1999)

\* phenomenological treatment

- 3D: Arita, Kuroki, and Aoki (1999)

\* Hubbard model plus perturbation theory.

\*  $d (x^2 - y^2)$  and  $d (3z^2 - r^2)$  degeneracy for cubic  
lattices



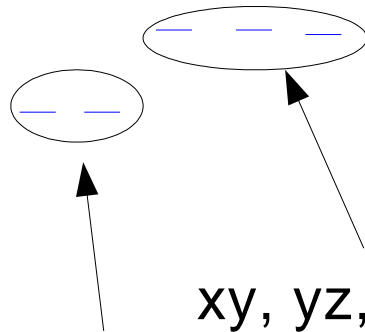
FM Grosche (2000)

# Lattice symmetry and d-wave pairing

Energy levels in free space (weak lattice potential)

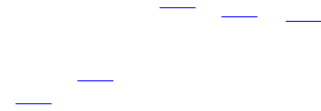


Energy levels in a cubic environment.



$(x^2 - y^2), (3z^2 - r^2)$

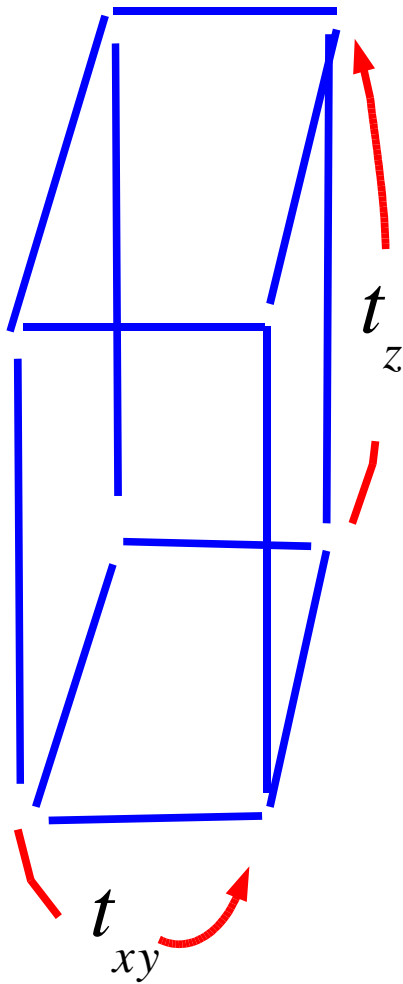
Energy levels in a nearly cubic environment



Ginzburg-Landau theory: constraints on the phase diagram

- For cubic symmetry with  $(x^2 - y^2), (3z^2 - r^2)$  degeneracy
  - \*  $\phi = (x^2 - y^2), (3z^2 - r^2), (x^2 - y^2) \pm (3z^2 - r^2), (x^2 - y^2) \pm i (3z^2 - r^2)$  are possible solutions
  - \* Details of system determine solutions, i.e. microscopic considerations
  - \* BCS-like phenomenology (weak-coupling) favors  $(x^2 - y^2) \pm i (3z^2 - r^2)$
  
- Tetragonal distortions lift the degeneracy
  - \*  $\phi = (x^2 - y^2)$  for quasi-2D conduction (xy)
  - \*  $\phi = (3z^2 - r^2)$  for quasi-1D conduction (z)
  - \* Possible second transition to, for example,  $\phi = (x^2 - y^2) \pm i (3z^2 - r^2)$  when the lattice is nearly cubic

# Method and model

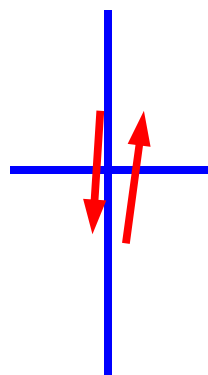


$$2D: t_z / t_{xy} = 0$$

$$3D: t_z / t_{xy} = 1$$

$$1D: t_z / t_{xy} \gg 1$$

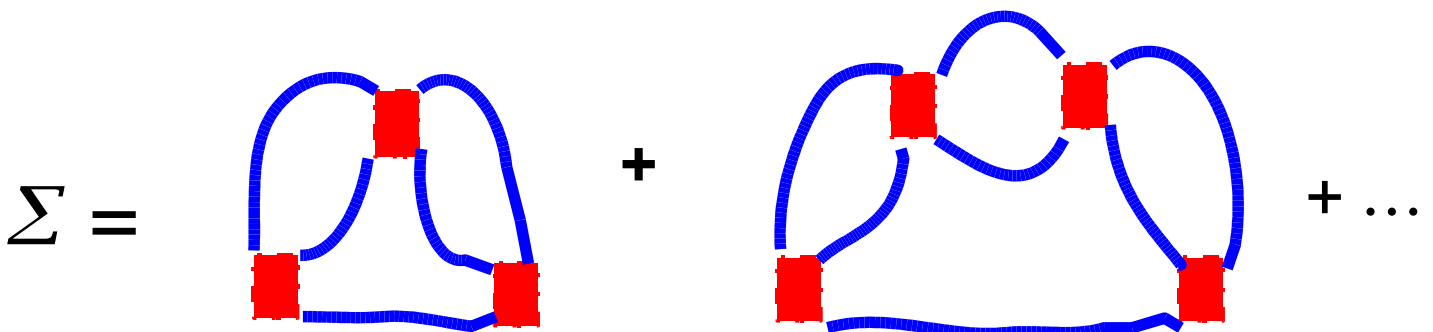
## Hubbard model



Potential energy increases by  $U$  for each doubly-occupied site.

FLEX approximation: Bickers, Scalapino and White (1987)

- Magnetic correlations --> electron pairing
- No fluctuations of d-wave pairing states (finite  $T_c$  in 2D)



# Method and model

Self-consistency:  $\Sigma \leftrightarrow G$

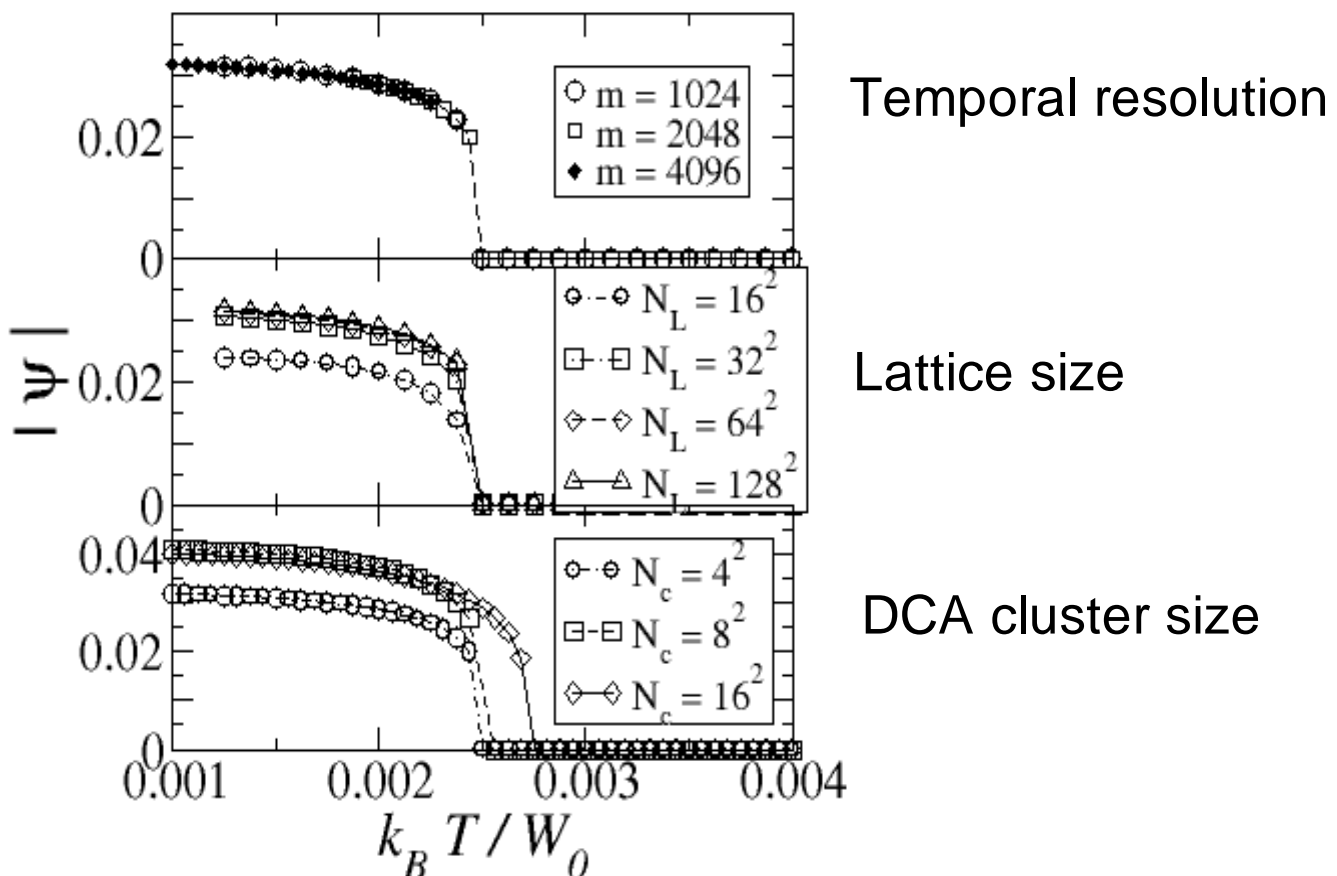
- 100 to 10,000 iterations per calculation.
- Adaptive mixing ratio between old and new solutions

Temporal (frequency) resolution:

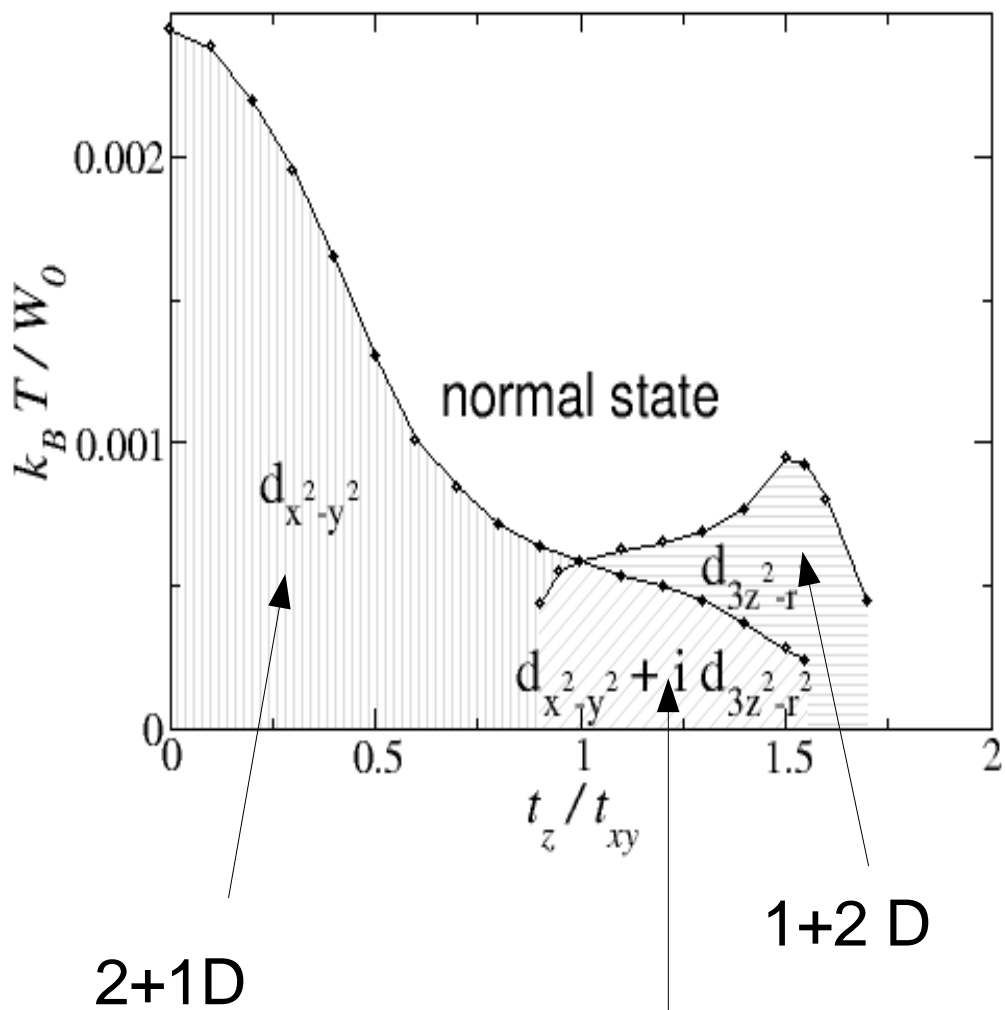
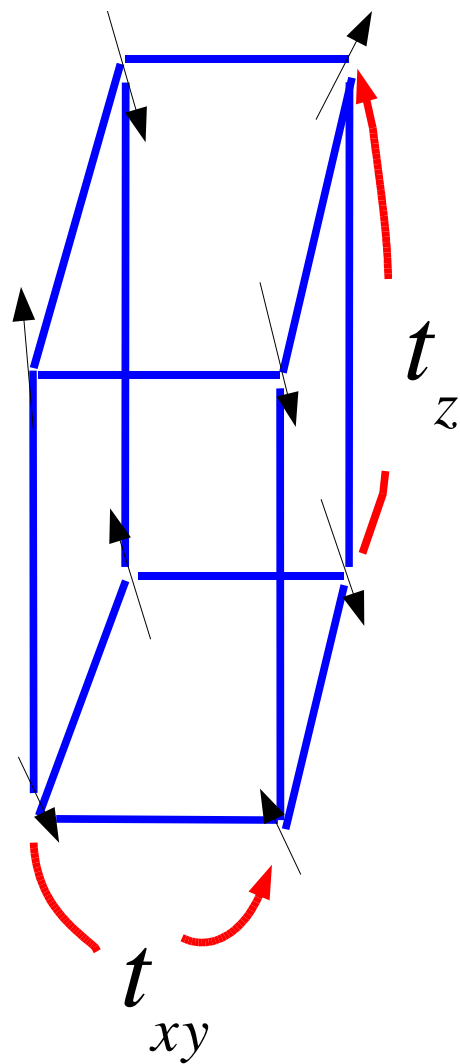
- Scales like  $1/T$  ( $T$ =temperature)
- As many as 16384 time/frequency points used at low  $T$
- Analytic treatment of high frequencies.

Lattice size :

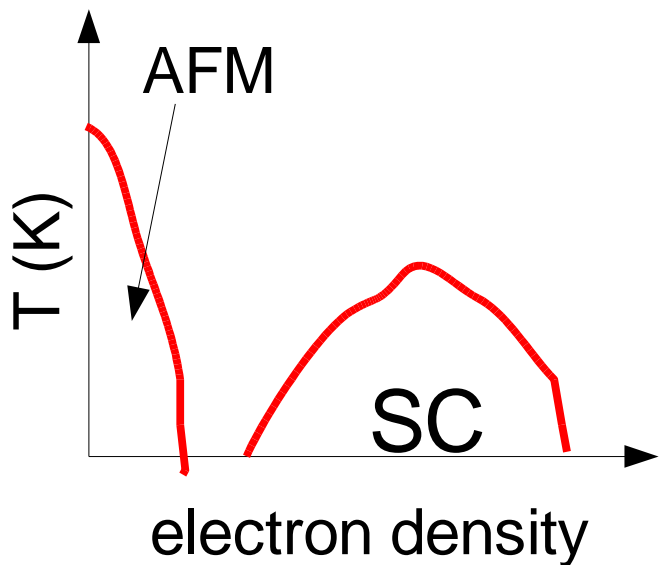
- Needs to be at least  $32 \times 32 \times 32$  to represent  $L \rightarrow \infty$  limit
- Use DCA method of Jarrell and collaborators to estimate correlation effects on  $4 \times 4 \times 4$  lattices.



# Upshot: possible phase diagram for AFM-mediated superconductivity



3D: T-breaking



# Summary

- Calculated phase diagram for anisotropic Hubbard model
- “Novel” phase diagram in the vicinity of cubic symmetry

## Future work

- p states in strontium ruthenate:  $p_x + i p_y$
- Model sensitivity (density variations, hopping range)
- Thermodynamics (magnetic penetration depth, specific heat, coherence length)
- Disorder