Fermion Glue in the Hubbard Model: New Insights into the Cuprate Pairing Mechanism with Advanced Computing

Presented by

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SC07

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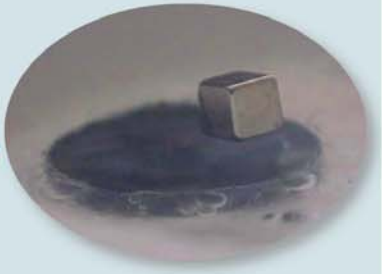
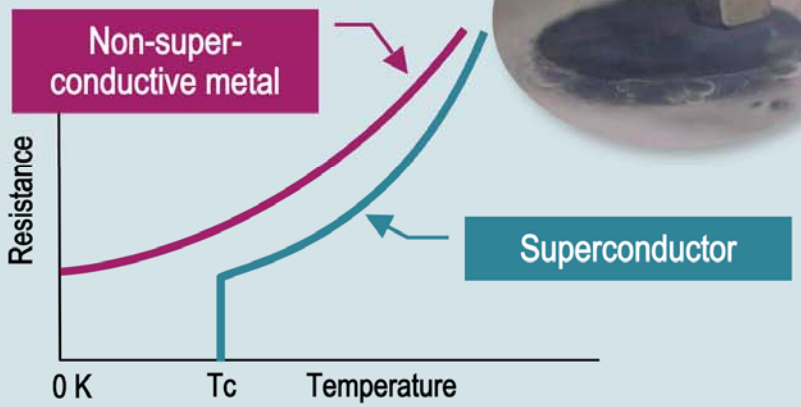
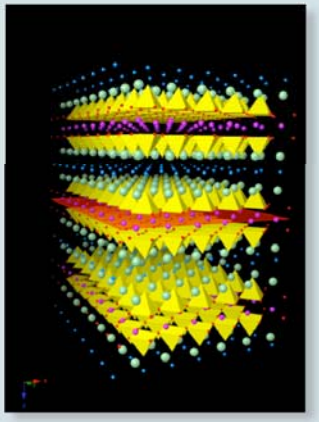
Outline

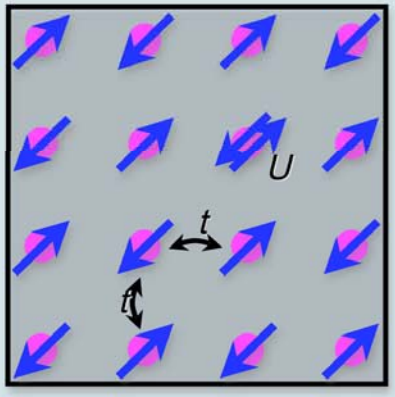
Superconductivity





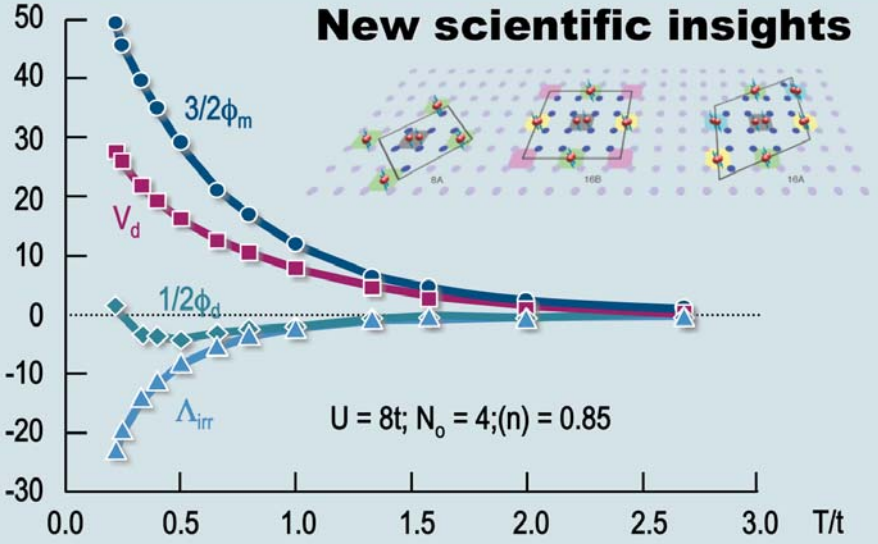
A model for high-temperature superconductors





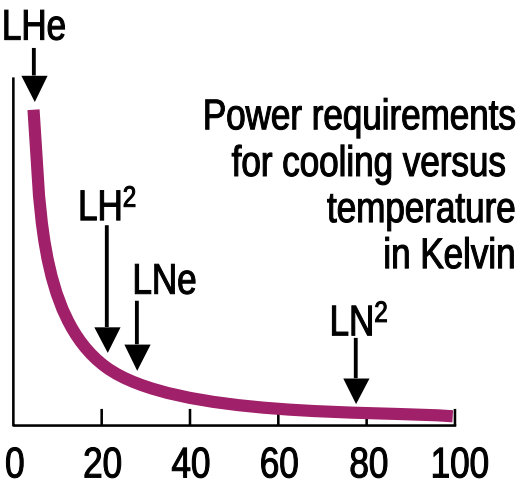
Algorithm and leadership computing

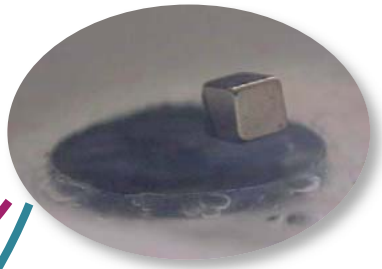
New scientific insights

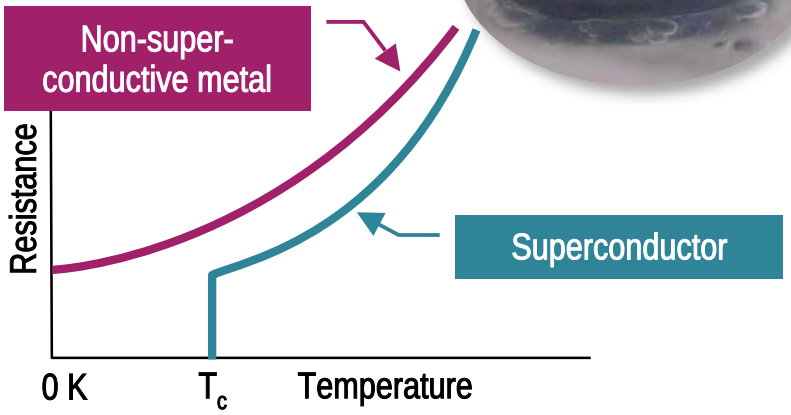


What is superconductivity?

- A macroscopic quantum state with
  - Zero resistance
  - Perfect diamagnetism
- Applications:
  - MAGLEV, MRI, power transmission, generators, motors
- Only disadvantage:
  - Cooling necessary
  - $T_c \approx 150$ K in HTSC
- Ultimate goal:
  - $T_c \approx$ room temperature

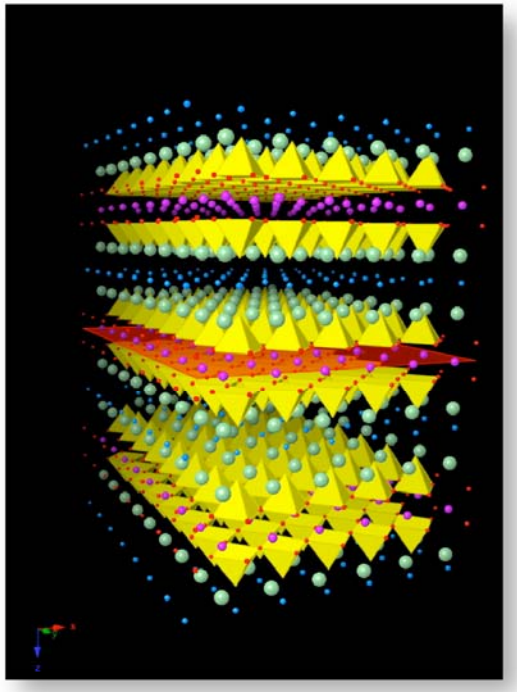




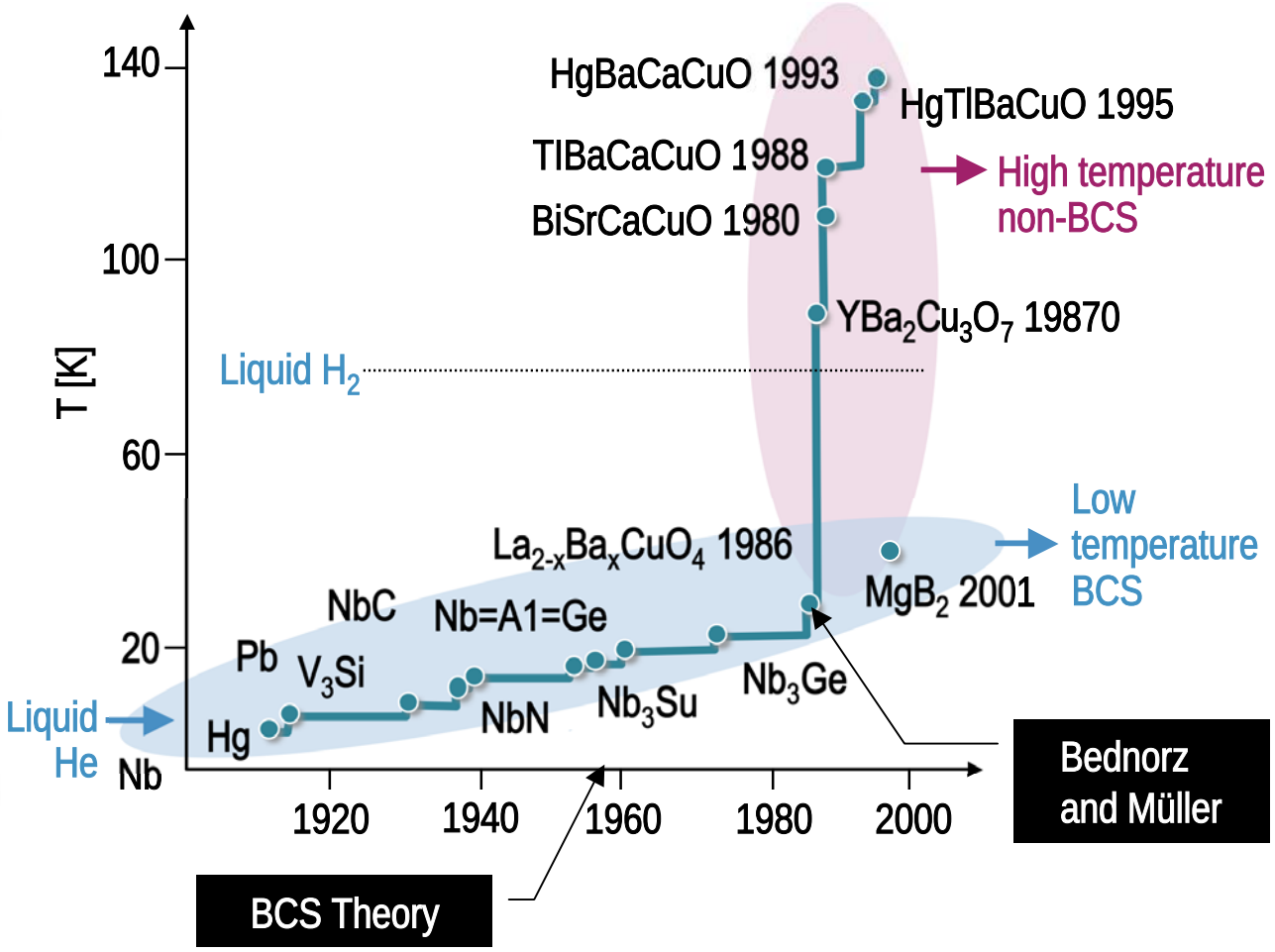


High-temperature superconductors

Discovered by
Bednorz and Müller
in 1986

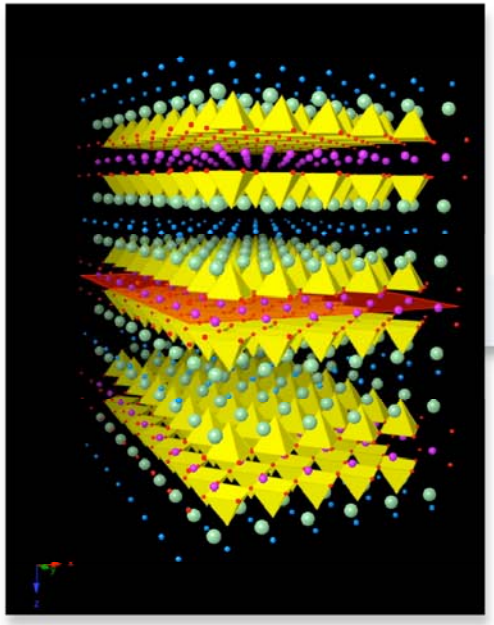


- Highly anisotropic
- Superconducting CuO planes

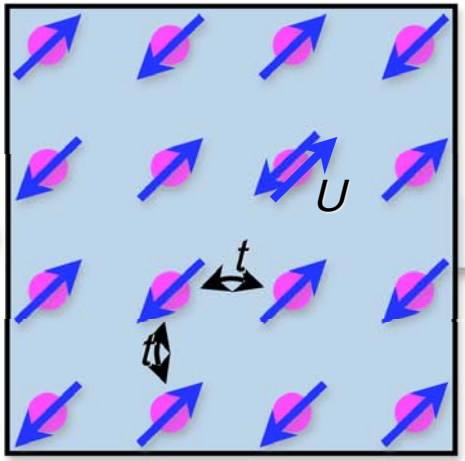


2-D Hubbard model of high-temperature superconductors

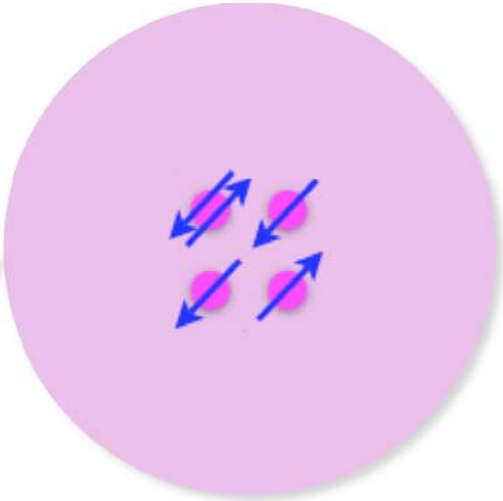
HTSC: 10^{23} interacting electrons



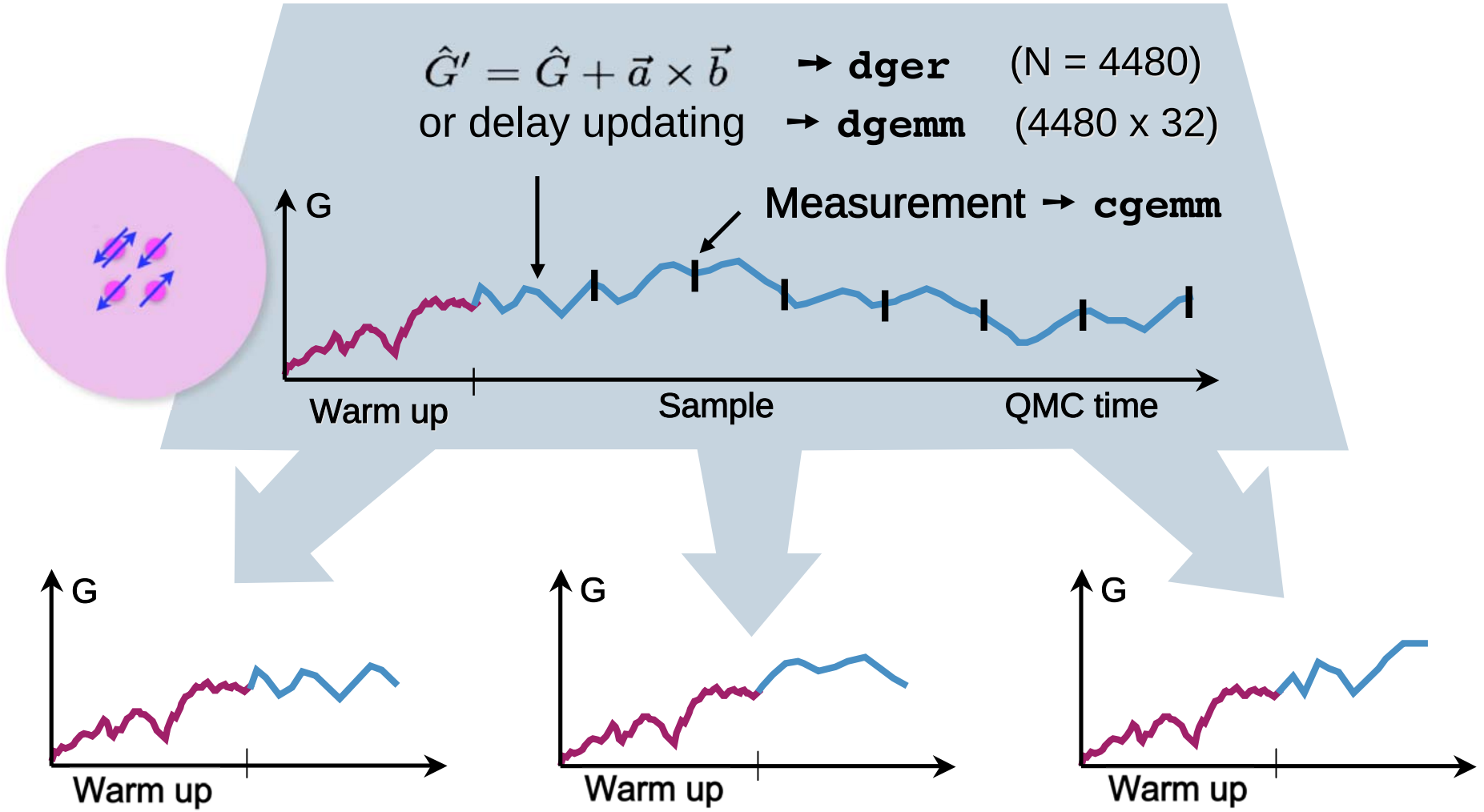
2-D Hubbard model for CuO planes



DCA/QMC: Map Hubbard model onto embedded cluster



Algorithm and leadership computing:
Fixed startup cost favors fewer, faster processors → Cray X1E



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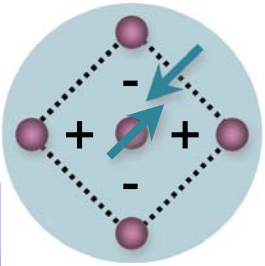
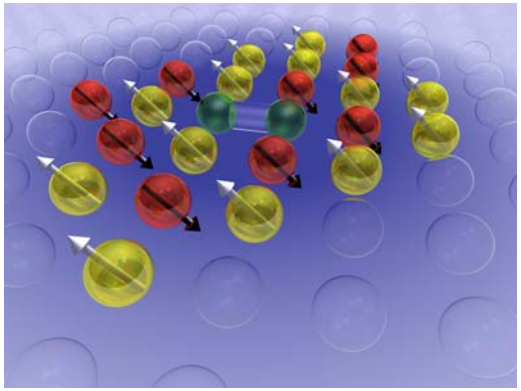
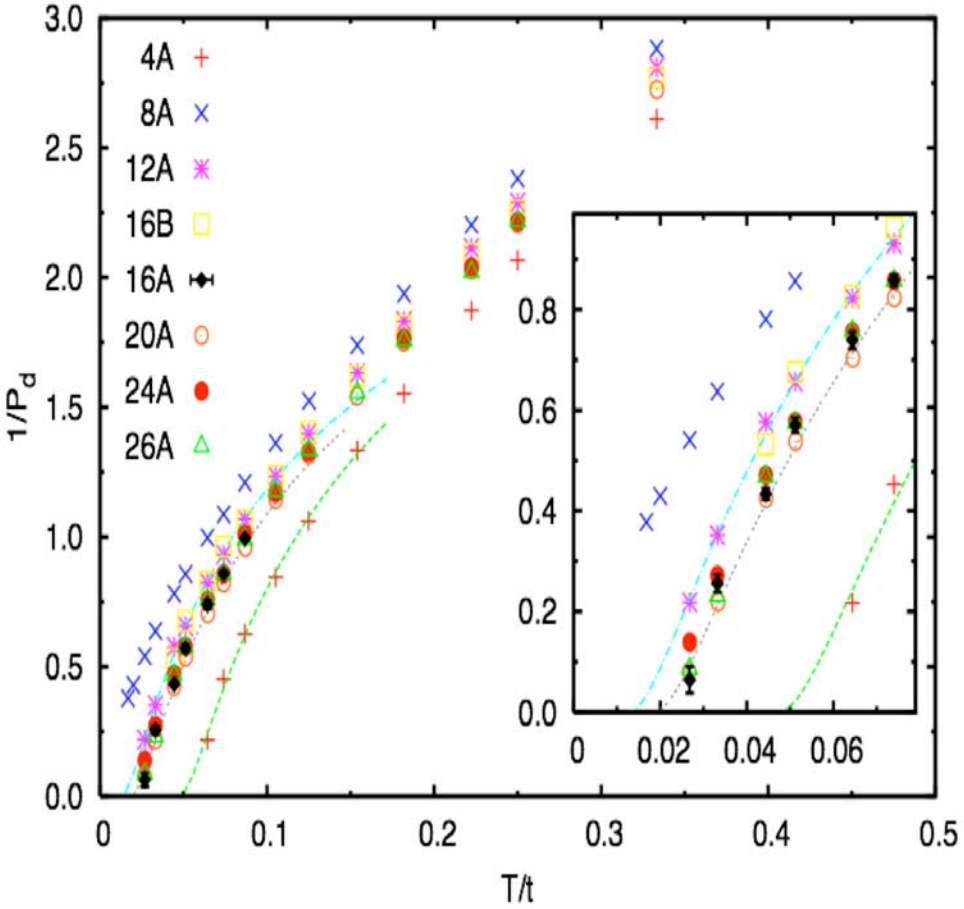
Superconductivity as a consequence of strong electronic correlations



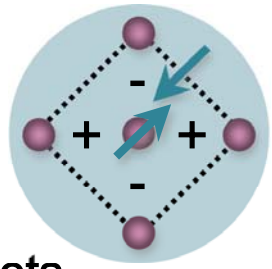


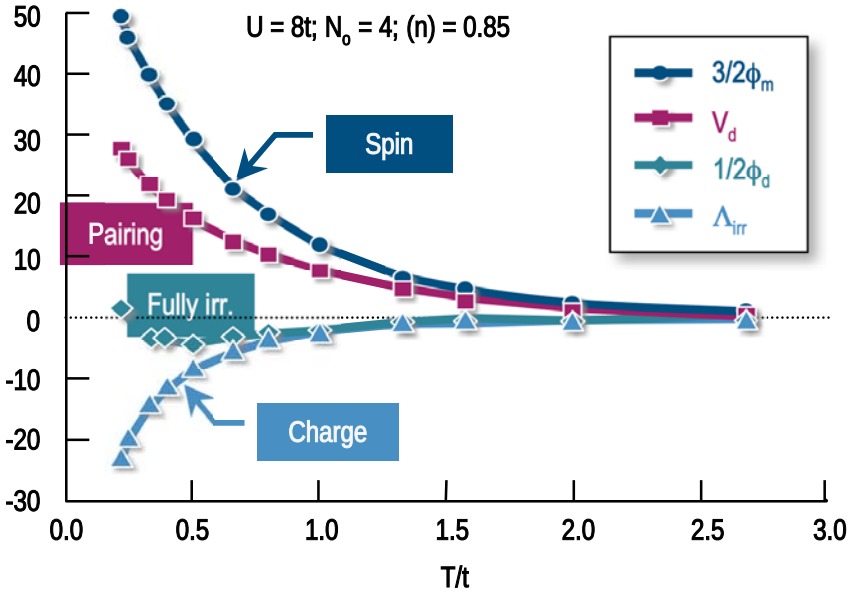


N_c	Z_d	T_c
4A	0	0.056
8A	1	-0.006
12A	2	0.016
16B	2	0.015
16A	3	0.025
20A	4	0.022
24A	4	0.020
26A	4	0.023

T. A. Maier, M. Jarrell, T. C. Schulthess, P. R. C. Kent, J. B. White, Systematic study of D-wave superconductivity in the 2D repulsive Hubbard model, *Phys. Rev. Lett.* **95**, 237001 (2005).

Magnetic origin of pairing interaction



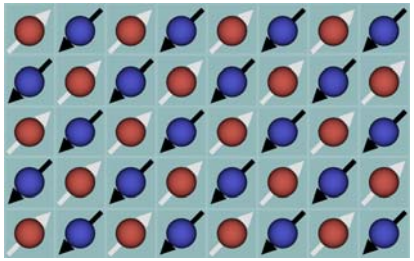


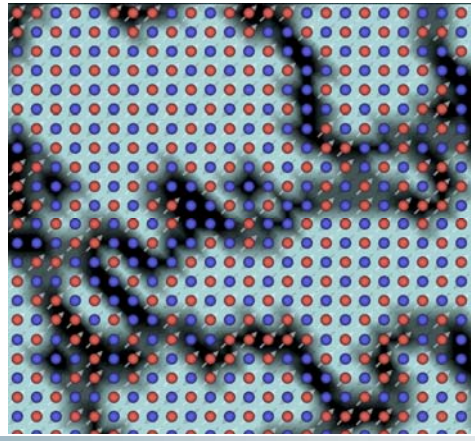
- Attractive pairing interaction between nearest neighbor singlets
- Dynamics associated with antiferromagnetic spin fluctuation spectrum
- Pairing interaction mediated by antiferromagnetic fluctuations

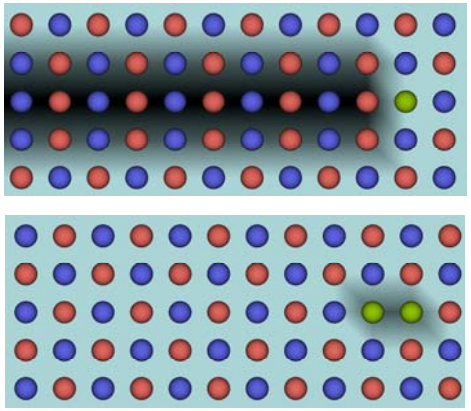
T. A. Maier, M. S. Jarrell, and D. J. Scalapino, Structure of the pairing interaction in the two-dimensional Hubbard Model, *Phys. Rev. Lett.* **96**, 047005 (2006).

T. A. Maier, M. Jarrell, and D. J. Scalapino, Pairing interaction in the two-dimensional Hubbard model studied with a dynamic cluster quantum Monte Carlo approximation, *Phys. Rev. B,* **74**, 094513 (2006).

T. A. Maier, M. Jarrell, and D. J. Scalapino, Spin susceptibility representation of the pairing interaction for the two-dimensional Hubbard model, *Phys. Rev. B*, **75**, 134519 (2007).





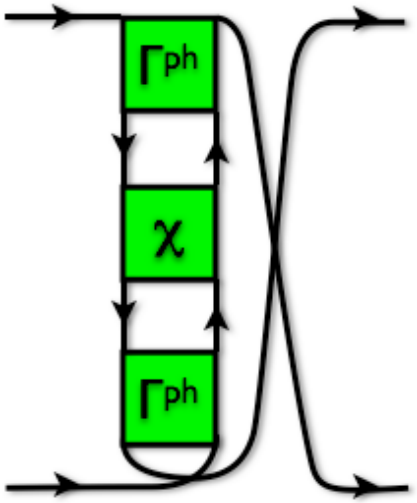


Spin susceptibility representation enables neutron scattering validation

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

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

Electron filling	<n>	0.95	0.90	0.85
"Exact" QMC	T_{c0}	0.080	0.074	0.067
Ū fitted from pairing interaction	$T_{c0}^{(1)}$	0.100 (25%)	0.087 (18%)	0.074 (10%)
Ū fitted from single-particle spectrum	$T_{c0}^{(2)}$	0.108 (35%)	0.084 (14%)	0.064 (4%)



T. A. Maier, A. Macridin, M. Jarrell and D. J. Scalapino, Systematic analysis of a spin susceptibility representation of the pairing interaction in the 2D Hubbard Model, *Phys. Rev. B*, in press (2007).

- Future: Demonstrate validity of Hubbard model simulations
  - Measure spin susceptibility in neutron scattering experiments and calculate T_c

Summary/conclusions/outlook

- Superconductivity: A macroscopic quantum effect
- 2-D Hubbard model for strongly correlated high-temperature superconducting cuprates
- Dynamic cluster quantum Monte Carlo simulations on Cray X1E
- Superconductivity as a result of strong correlations
- Pairing mediated by antiferromagnetic spin fluctuations
- Simple spin susceptibility representation of pairing interaction
- Verification by neutron scattering experiments?

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