Pairing in multi-Fermi-surface systems: New insight into unconventional superconductivity with advanced computing

Presented by

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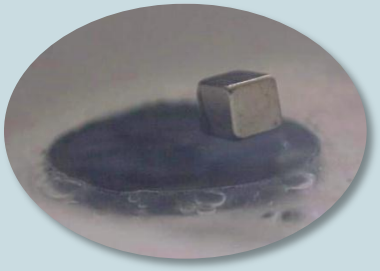
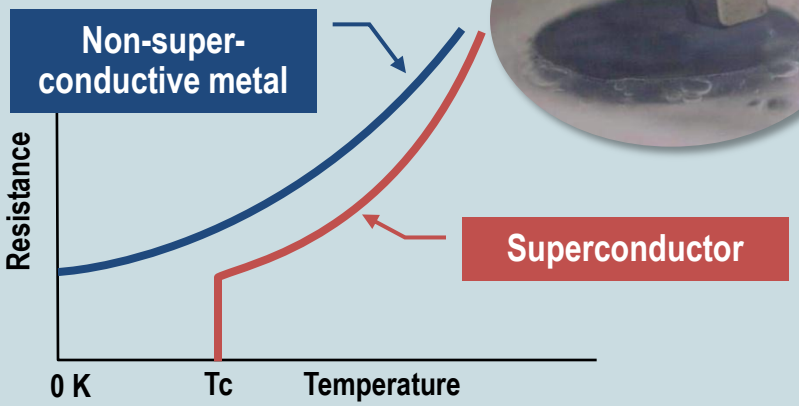
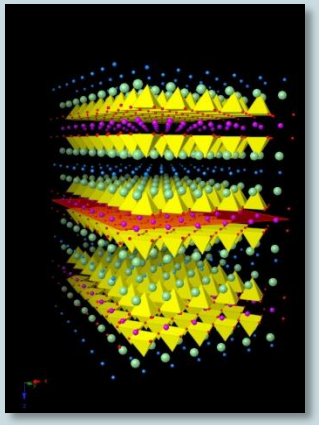
Outline

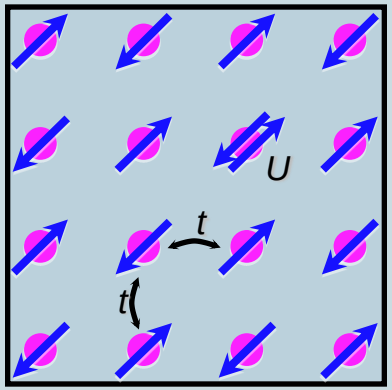
Superconductivity





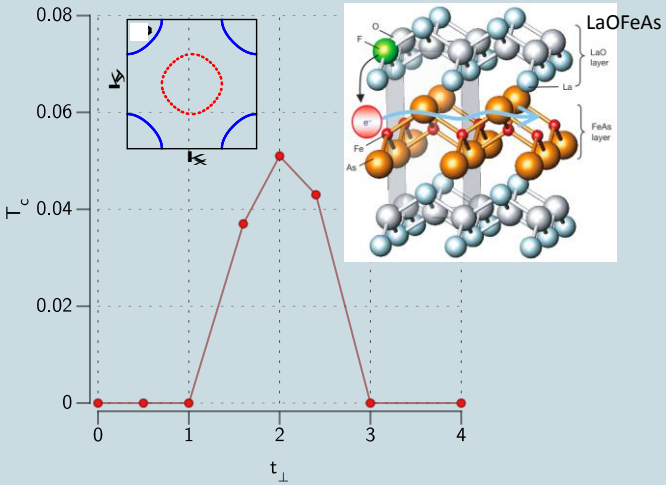
A model for high temperature superconductors





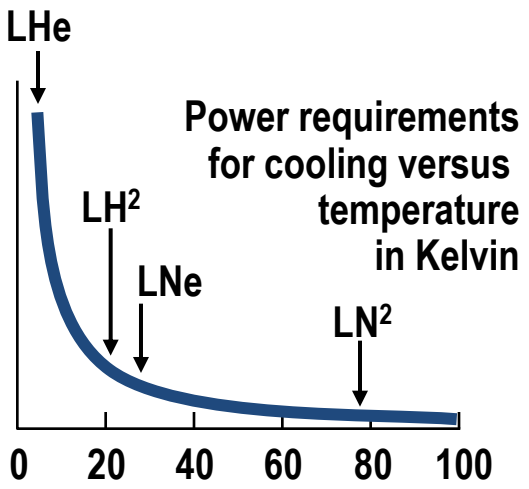
Algorithm and leadership computing

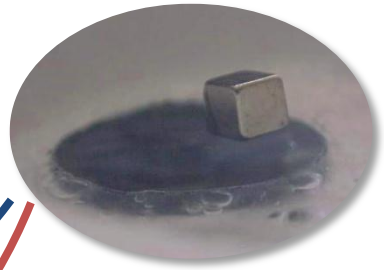
New scientific insights

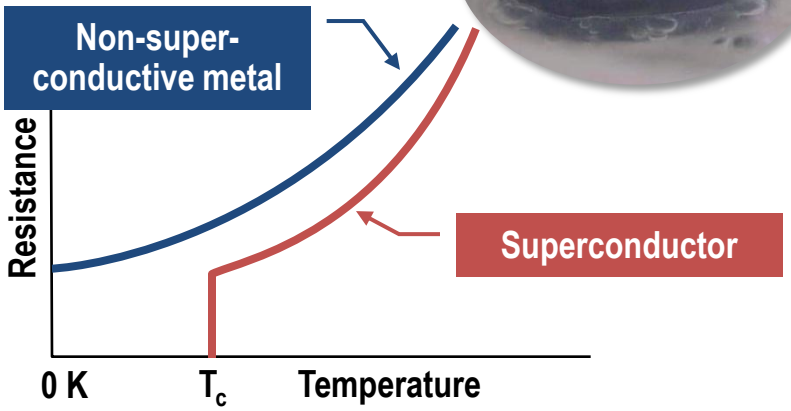


What is superconductivity?

- 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 high temperature superconductivity
- Ultimate goal
  - $T_c \approx$ room temperature

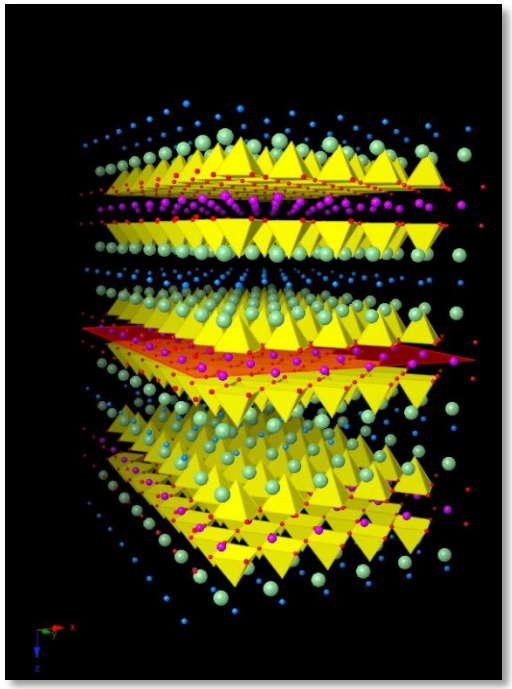




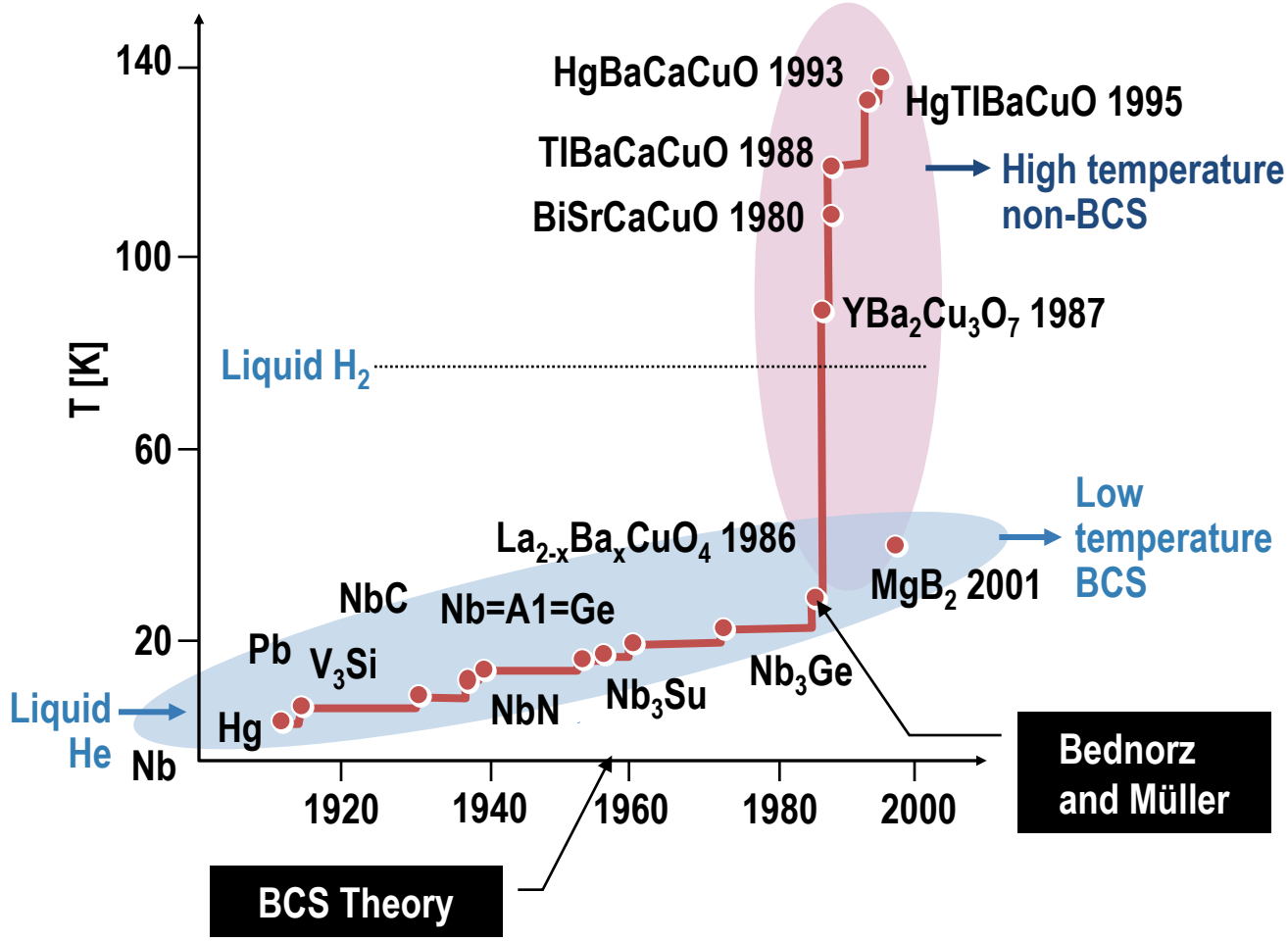


High temperature superconductors

- Discovered by Bednorz and Müller in 1986

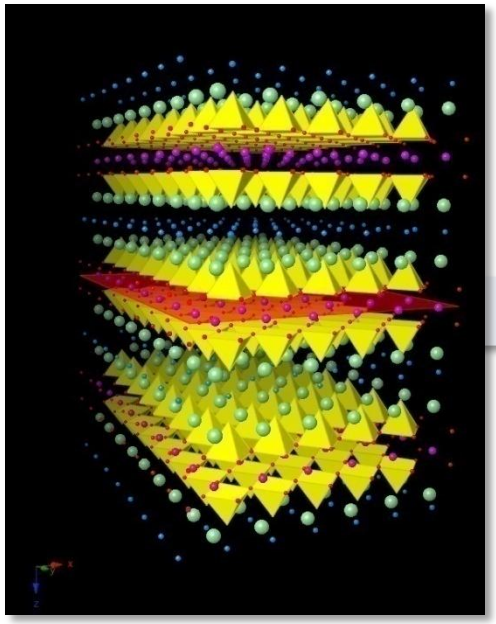


- Highly anisotropic
- Superconducting CuO planes

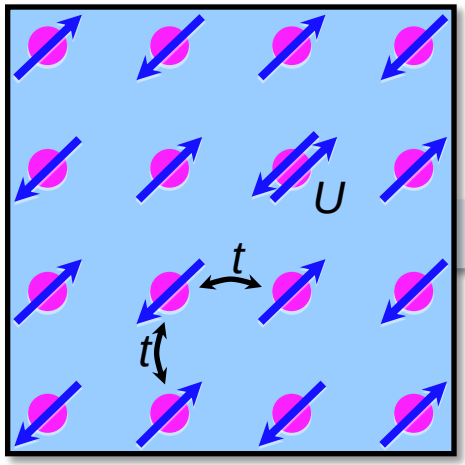


2D Hubbard model of high temperature superconductors

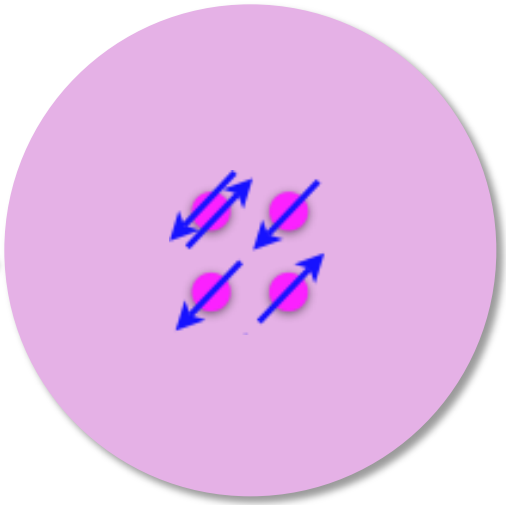
HTSC: 10^{23} interacting electrons



2D Hubbard model for CuO planes

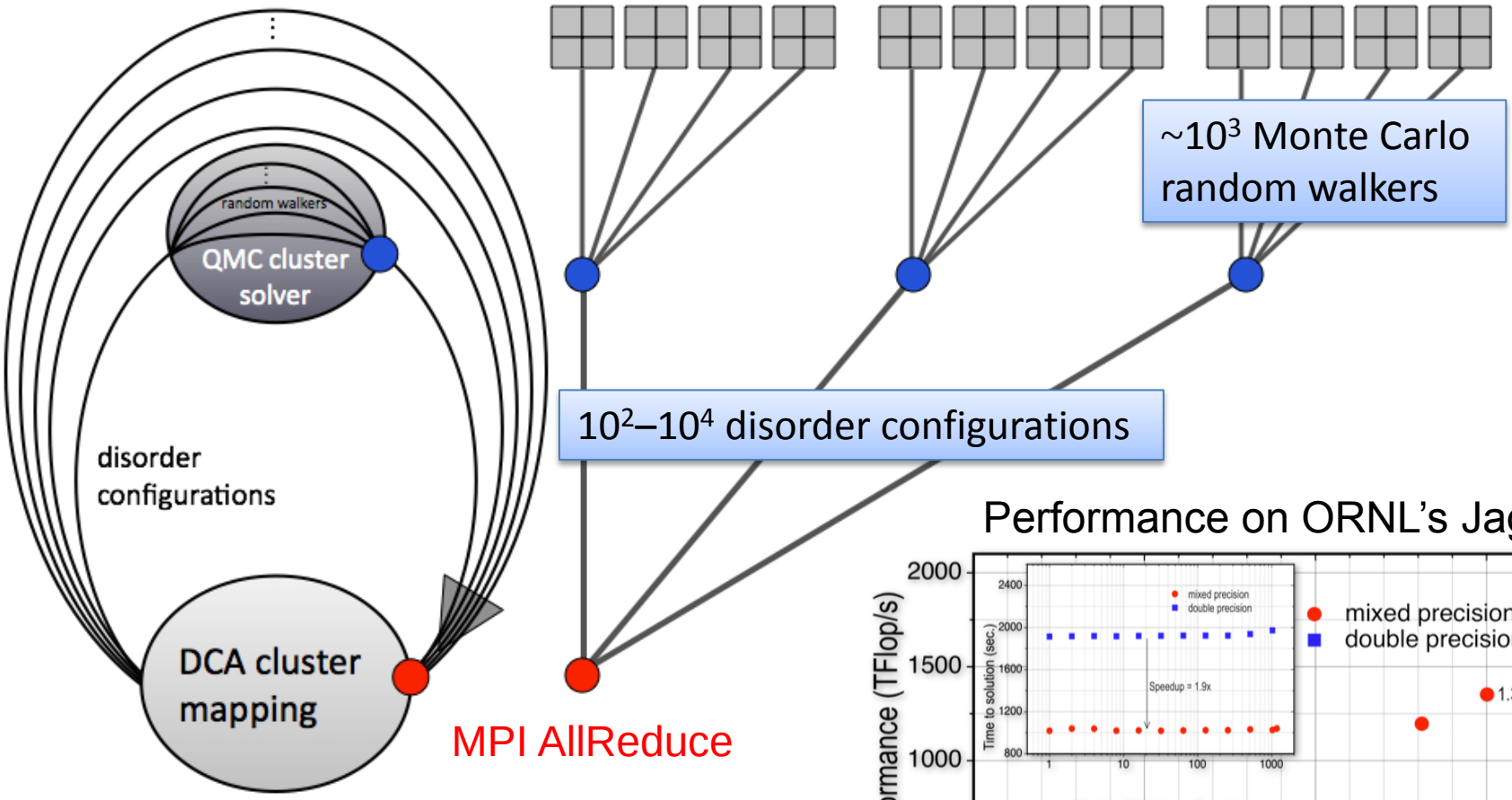


DCA/QMC: Map Hubbard model onto embedded cluster

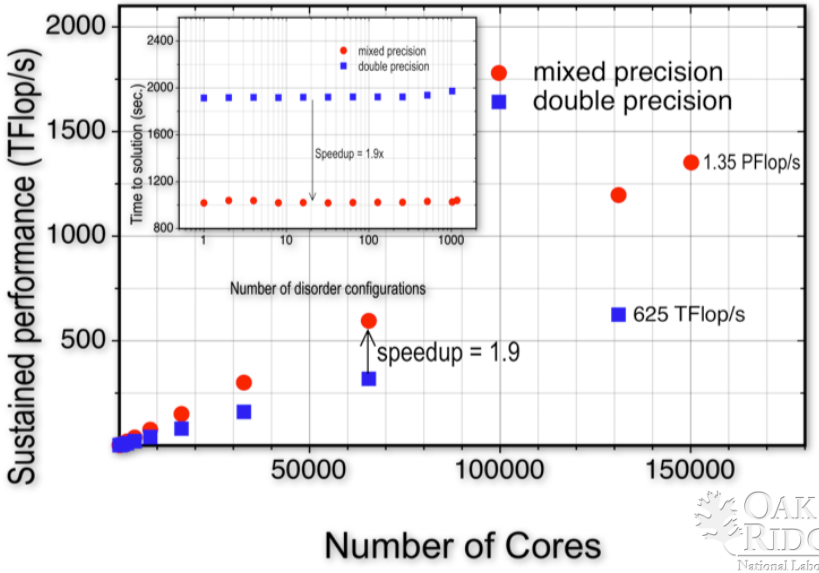


Solve effective cluster problem with quantum Monte Carlo

Algorithm and leadership computing:
Concurrency, scaling and efficiency of DCA++



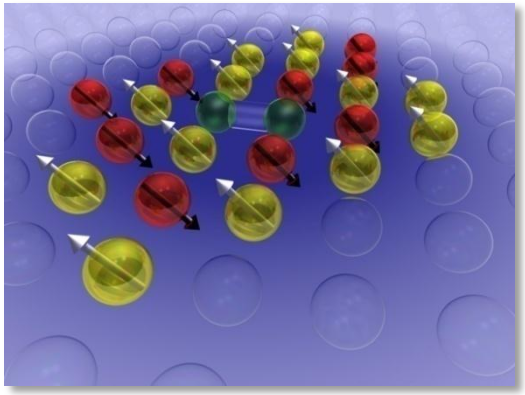
Performance on ORNL's Jaguar



2008 Gordon Bell prize winner for sustained performance

Fermion glue in the Hubbard model: Spin-fluctuation mediated pairing

- **Extensive simulations show that antiferromagnetic spin fluctuations cause electrons to join into Cooper pairs and cause superconductivity in the 2D Hubbard model**



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)

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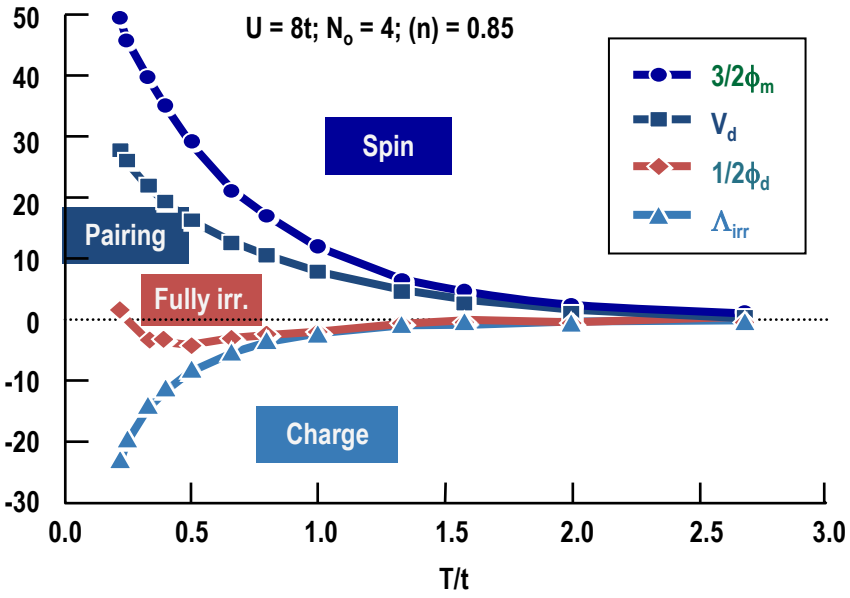
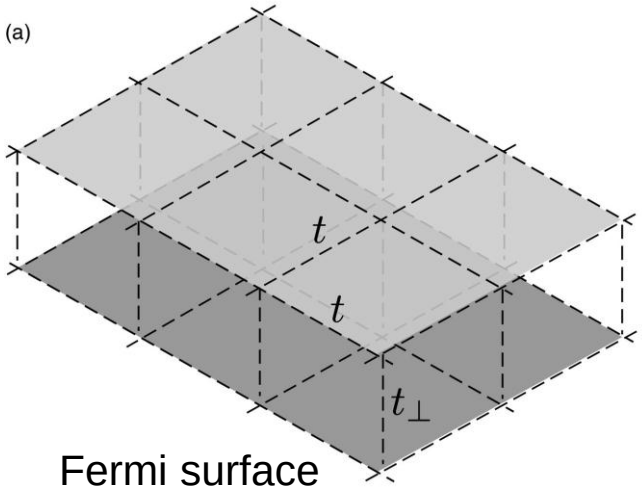
T. A. Maier, M. Jarrell, and D. J. Scalapino, Spin susceptibility representation of the pairing interaction for the two-dimensional Hubbard model, *Phys. Rev. B* **75**, 134519 (2007)

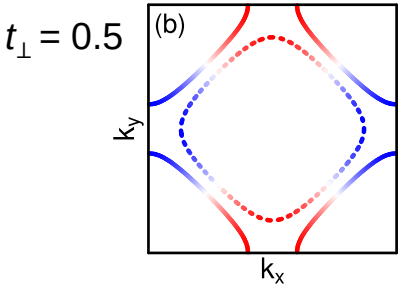
T. A. Maier, D. Poilblanc, and D. J. Scalapino, Dynamics of the pairing interaction in the Hubbard and t-J models of high-temperature superconductors, *Phys. Rev. Lett.* **100**, 237001 (2008)

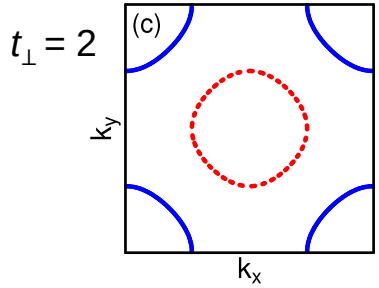


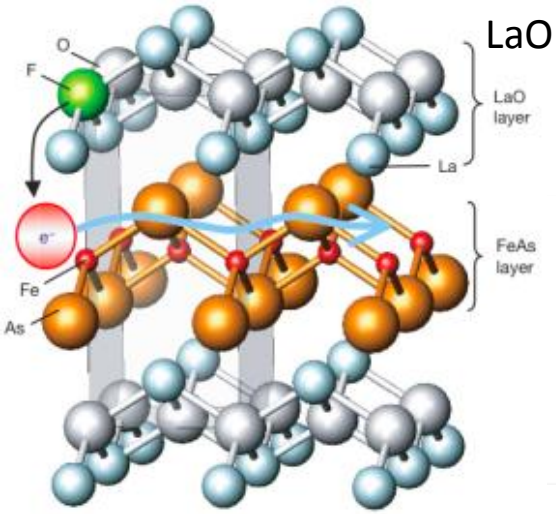
Bi-layer Hubbard model — Multiple Fermi surfaces as in Fe-pnictides



Fermi surface

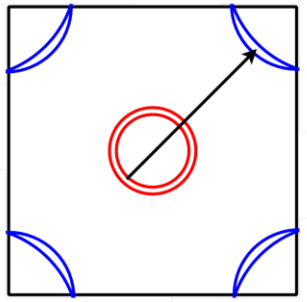






LaOFeAs

Fe-pnictide Fermi surface

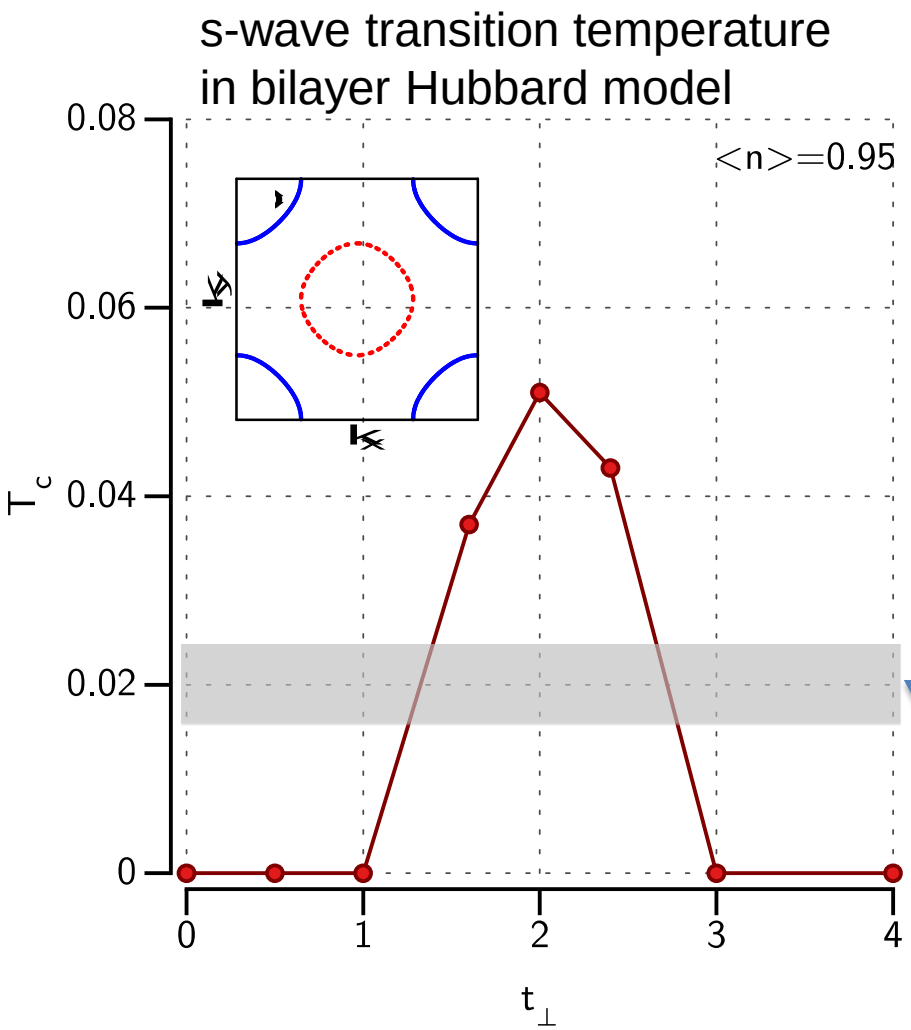


Bi-layer Hubbard model:

— Allows to study superconductivity in system with multiple Fermi surfaces

— Leading correlations can be tuned from antiferromagnetic to valence bond singlets with increasing $t_\perp$

Sign-changing s-wave superconductivity with high T_c



High T_c through large inter-layer spin-fluctuation pairing interaction and simultaneous avoidance of Mott quasiparticle degradation

Maximum d-wave transition temperature in 2D single-layer Hubbard model

T. A. Maier & D.J. Scalapino, preprint arXiv:1107.0401.

Summary, conclusions, and outlook

- Superconductivity: A macroscopic quantum effect
- 2D Hubbard model for strongly correlated high temperature superconducting cuprates
- Dynamic cluster quantum Monte Carlo simulations on Cray XT4/XT5
- Superconductivity as a result of antiferromagnetic spin-fluctuations
- Bi-layer Hubbard model to study pairing in systems with multiple Fermi surfaces such as in Fe-pnictides
- Sign-changing s-wave superconductivity in bi-layer Hubbard model with very high T_c.

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