Decisive change in the understanding of high-temperature superconductivity through improved computing capability

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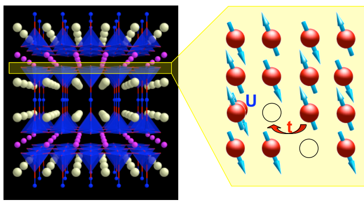
High-Tc superconductors & Model

Layered structure **2D Hubbard model**

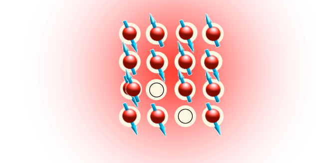


- Superconductivity takes place in CuO-planes → Reduction to 2D model
- CuO unit cell represented by single site → 2D Hubbard model:
  - N interacting electrons on a square lattice
  - Problem: $N \approx 10^{23}$
  - Exactly solvable only in 1D, not in 2D

Technique: DCA

- Cuprates: $U \sim t$ → no small parameter for perturbative expansion
- But: Length-scale of correlations small

→ Dynamical Cluster Approximation (DCA): Map system onto cluster embedded in mean-field

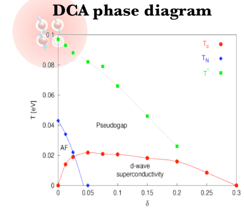


✓ Thermodynamic limit

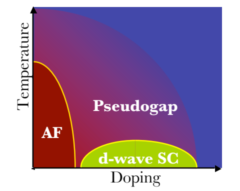
✓ Correlation within the cluster are treated explicitly, while those at longer length-scales are treated on the mean-field level

4-site cluster DCA results

DCA phase diagram



Generic HTSC phase diagram



✓ Antiferromagnetic and d-wave superconducting phase, pseudogap behavior in normal state

✗ But: Results contradict Mermin-Wagner theorem:

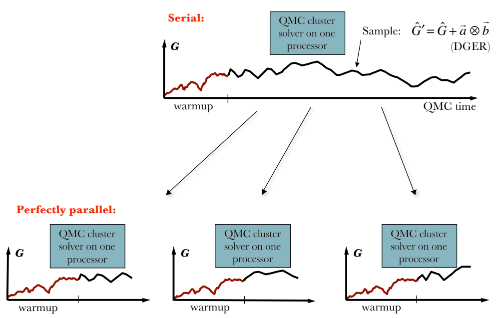
No finite T transition in 2D systems to state with broken continuous symmetry

→ No antiferromagnetism, superconductivity only as topological Kosterlitz-Thouless order at finite T.

- Violation due to small cluster size → Larger cluster studies necessary! But computational cost grows like N_c^3.

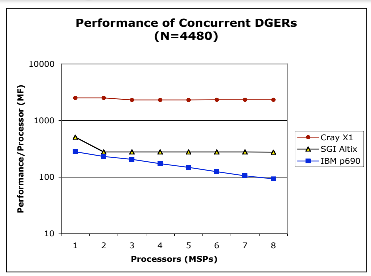
DCA/QMC code: Perfectly parallel?

Take independent measurements of observables along Markov-chain in QMC time → perfectly parallel



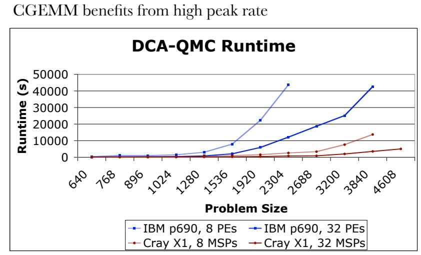
- But: Fixed startup cost on every processor

DCA/QMC code: Performance



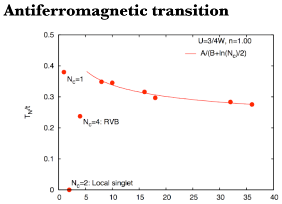
- Production runs on Cray X1 (at ~50% efficiency) perform up to 25 times faster than on IBM Power4
- Cray X1 enables simulations of larger clusters
  - High memory bandwidth
  - Powerful processors

- Fixed startup cost favors fewer faster processors
- Rank-1 matrix update (DGER)
  - Few floating point operations per memory operation
  - requires high memory bandwidth
- CGEMM benefits from high peak rate



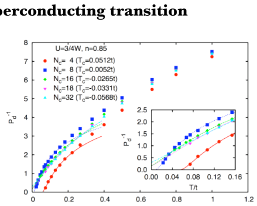
Large cluster DCA results

Antiferromagnetic transition



✓ Transition temperature falls logarithmically with cluster size → Mermin-Wanger theorem recovered in large cluster limit

Superconducting transition

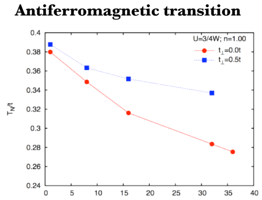


- Inverse pair-field susceptibility crosses zero for N_c=4 and 8 → superconducting transition

✗ Low T extrapolation for larger N_c: No finite T superconducting transition for N_c>8

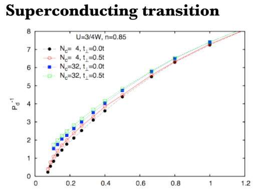
- Additional inter-planar coupling $t_{\perp}$ between infinite set of Hubbard planes treated in planar DCA approximation (no dynamics along c-axis)

Antiferromagnetic transition



✓ Antiferromagnetism stabilized with $t_{\perp}$

Superconducting transition



✗ Interplanar coupling does not stabilize superconductivity in larger clusters

Conclusions and future goals

Conclusions

- The Nc=4 mean-field DCA/QMC simulations of 2D Hubbard model represent an excellent description of the low-energy physics of the HTSC.
- The performance advantage of the Cray X1 provides the capability to perform simulations at much larger cluster sizes and lower temperatures, thus enabling new science.
- Consistent with the Mermin-Wagner theorem, the finite temperature antiferromagnetic and superconducting transitions found in the Nc=4 results are systematically suppressed with increasing cluster size.
- Most significantly, no Kosterlitz-Thouless superconducting transition is found in the large cluster results of the 2D Hubbard model at temperatures and dopings relevant to the cuprates.
- A simple, non-dynamical two-dimensional treatment of an additional inter-planar coupling between an infinite set of Hubbard layers is found to restore antiferromagnetism, but to have no effect on superconductivity.

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Future goals and computational requirements

- The large cluster DCA/QMC results show that the 2D Hubbard model lacks key ingredients to capture the physics of HTSC and hence call for a qualitatively different approach to solve the problem that has dominated condensed matter physics for almost two decades.

→ Some additional mechanism is necessary to stabilize the behavior seen in small clusters. Possibilities include

- Phonons
- Frustration
- Disorder (indications (chemical inhomogeneities) are seen in experiments)

New complexity

- Inclusion of disorder in the DCA/QMC simulations requires QMC sampling of many replicas of the cluster (one for each disorder realization).

Scalability = Capability

→ Many more processors are needed to tackle increased complexity