Impact of leadership computing on our understanding of strongly correlated electron systems

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Outline

- **Superconductivity: a short tutorial**
- **Single band 2-D Hubbard Model:**

  a new algorithm to solve the model
- **Why we need high memory bandwidth**
- **Results made possible by Cray X1**
- **Summary / Conclusions**

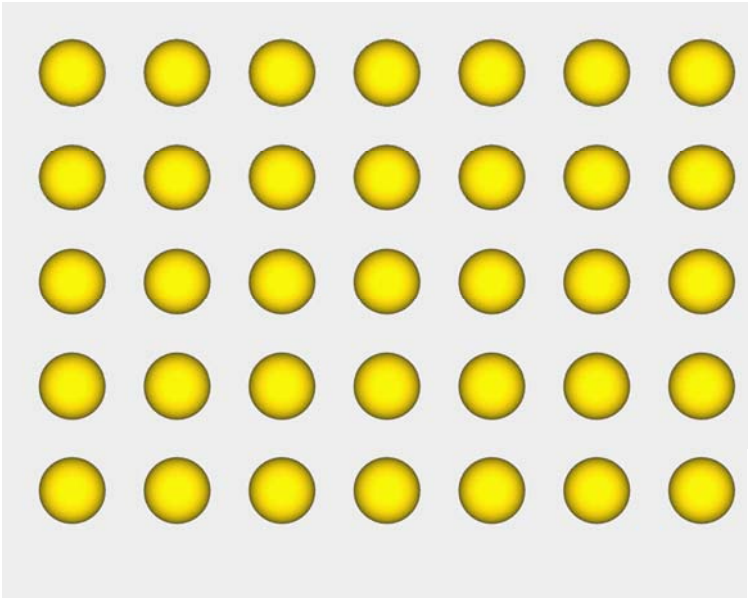
Superconductivity: what and what for

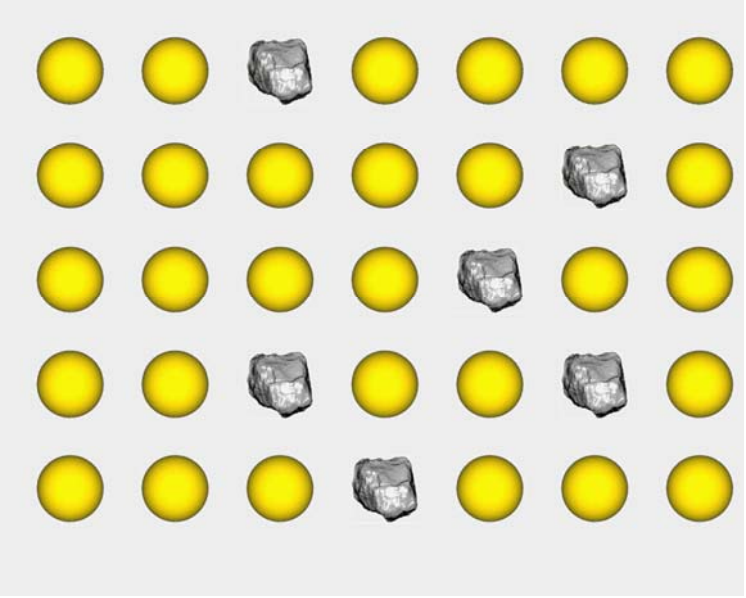
- **Zero resistance at finite (but low) temperatures**
  - **Discovered in 1911 by Kamerlingh-Onnes (Nobel Prize in 1913): Hg superconducting at 4.2 K**
  - **Later observed in other metals like Nb, Al, … but the critical temperature, T_c<23K**
- **Applications (examples):**

MRI (without need for liquid He cooling?)

Loss free power transmission (without cooling?)

Conduction in metals





- **Perfect metal at T=0K, resistance is zero**
- **Real metal at finite temperature:**
  - **scattering from defects, lattice vibrations, …**
  - **this leads to fluctuation in current,**
  - **which leads to dissipation (fluctuation dissipation theorem),**
  - **which is equivalent to a non vanishing resistance.**

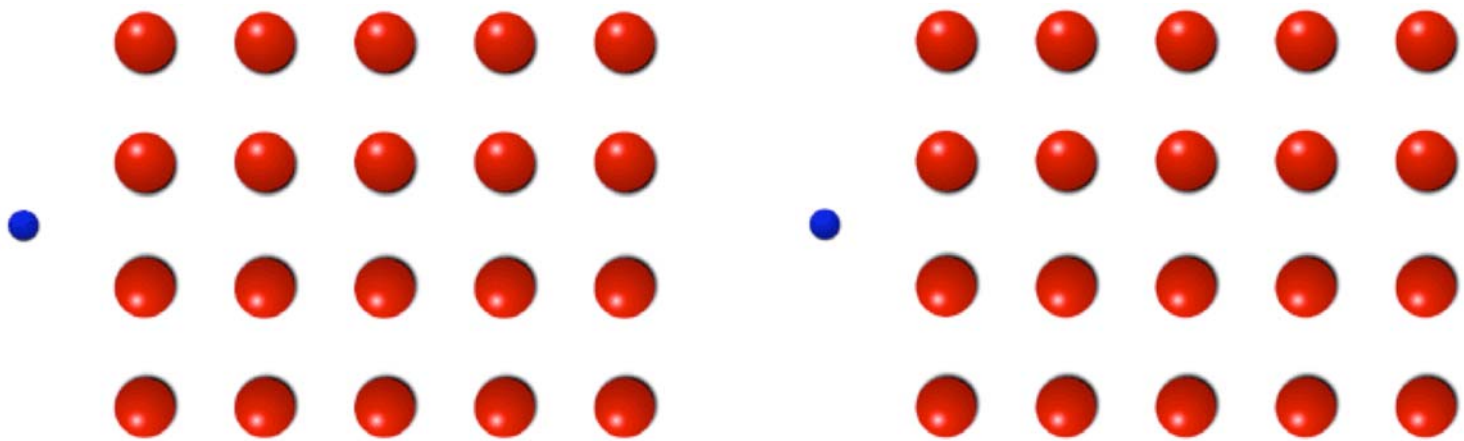
Fermions and Bosons in a nutshell

- **Quantum mechanical particles of one type are indistinguishable**
  - **All observable quantities have to symmetric**
- **Two types of particles in quantum mechanics:**
  - **Fermion**
    - **Wave function is anti-symmetric**
    - **Avoid each other (Pauli exclusion principle)**
  - **Bosons**
    - **Wave function if symmetric**
    - **Have tendency to condense into same state**

Electrons (and holes) are Fermions

BCS Pairing mechanism

- **When electrons form pairs, they behave like bosons and can condensed into a macroscopic quantum state**
- **Bardeen, Cooper, and Shriffer (BCS) develop rigorous description of pairing mechanism**
  - **Theory developed in the 1950s, Nobel Prize in 1973**



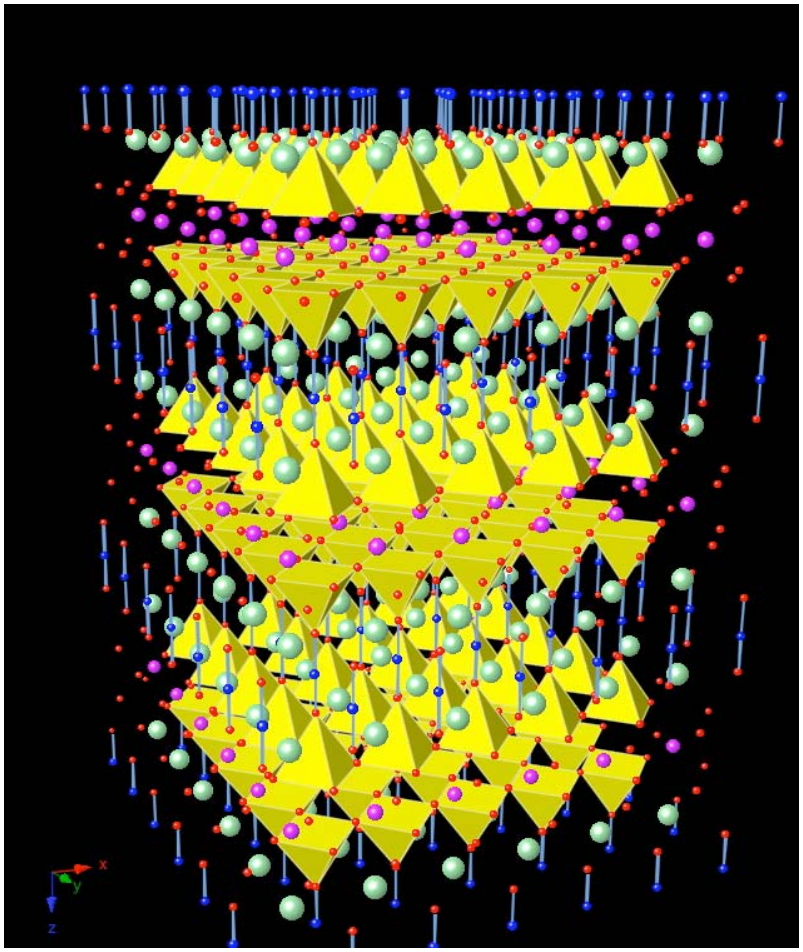
- **At T>20K, lattice vibration are strong and destroy pairs, superconductor becomes a normal metal.**

High Temperature Superconductivity

- **Doped $YBa_2Cu_3O_7$**
  - **Normal states is insulating / poor metal**
  - **Discovered to be a SC with T_c=30K in 1986 (75 years after Kamerlingh-Onnes)**
  - **1987 Nobel Prize for Bednorz and Muller**
  - **Within years, other transition metal oxides were discovered with T_c>100K (liquid Nitrogen cooled SC)**

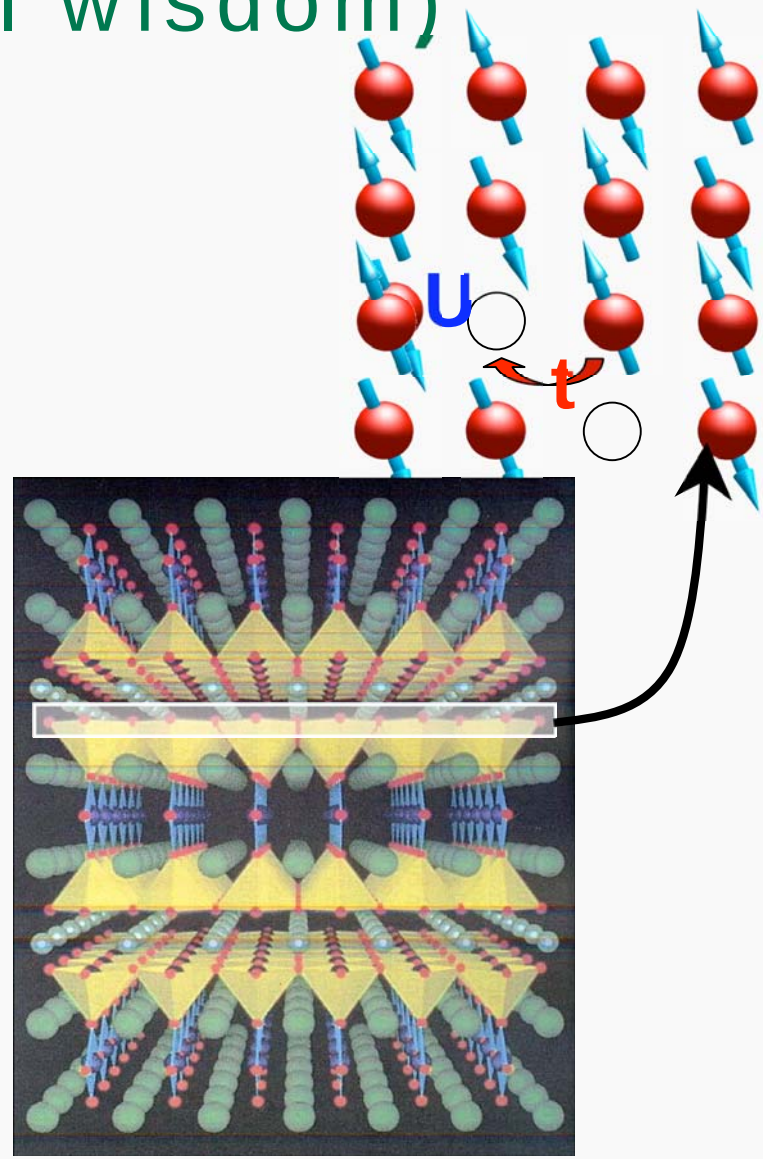
- **The daunting question of condensed matter physics today:**

  What is the mechanism responsible for pair formation in high temperature superconductors?



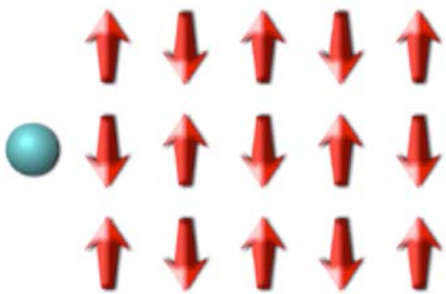
High Tc Superconductivity (conventional wisdom)

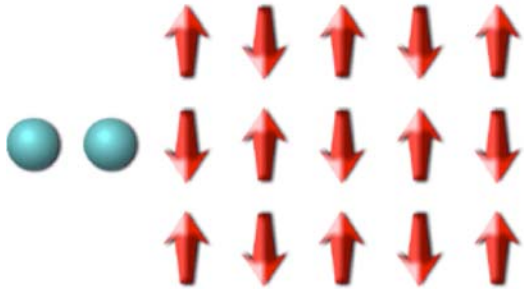
- **Model Copper oxide planes with single band 2D Hubbard models (Zhang & Rice, PRB 1989)**
- **Solvable only in 1-D not in 2-D!**
  - **Computationally very challenging: *N* interacting electrons on a lattice, where N ≈ 10^{23}**
- **David Pines: "arguably the major problem in physics today"**
  - **Over 1000 papers published per year over the last decade!**



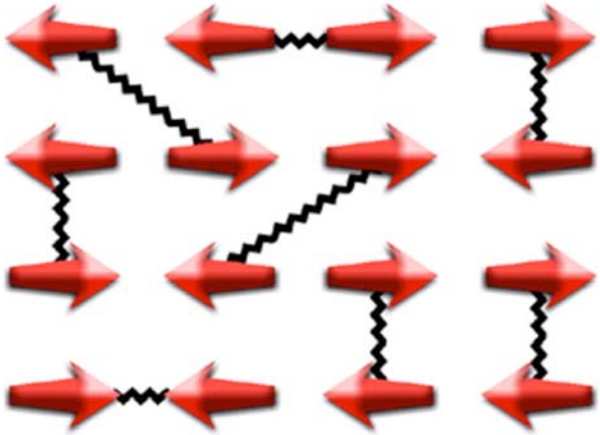
Many proposed paring mechanisms

- **Quasi particles in AF background (Hirsch 02)**





- **Resonating valence bond (Anderson 87)**



- **Computational solution ?**

The Computational Challenge

- **A macroscopic quantum effect:**

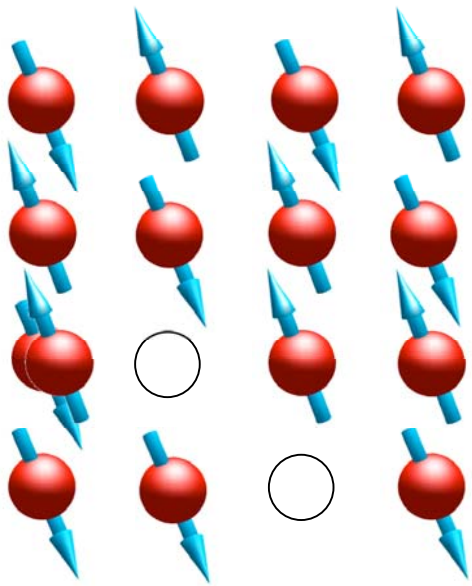
  ⇒**Account for ~10^{23} particles (thermodynamic limit)**

- **Strong correlation at atomic scale**

  ⇒**Explicitly account for microscopic interactions at the nano-scale**

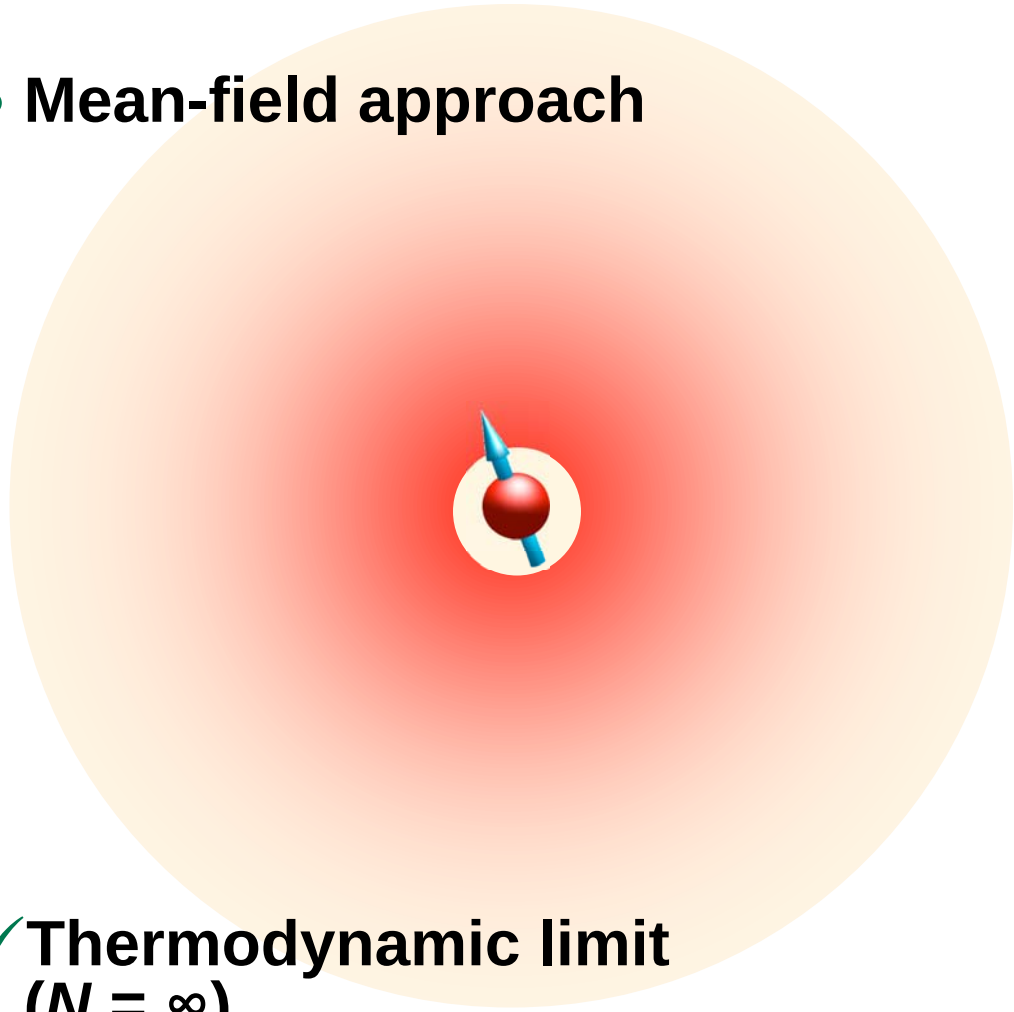
Computational Methods

- **Finite size simulations**



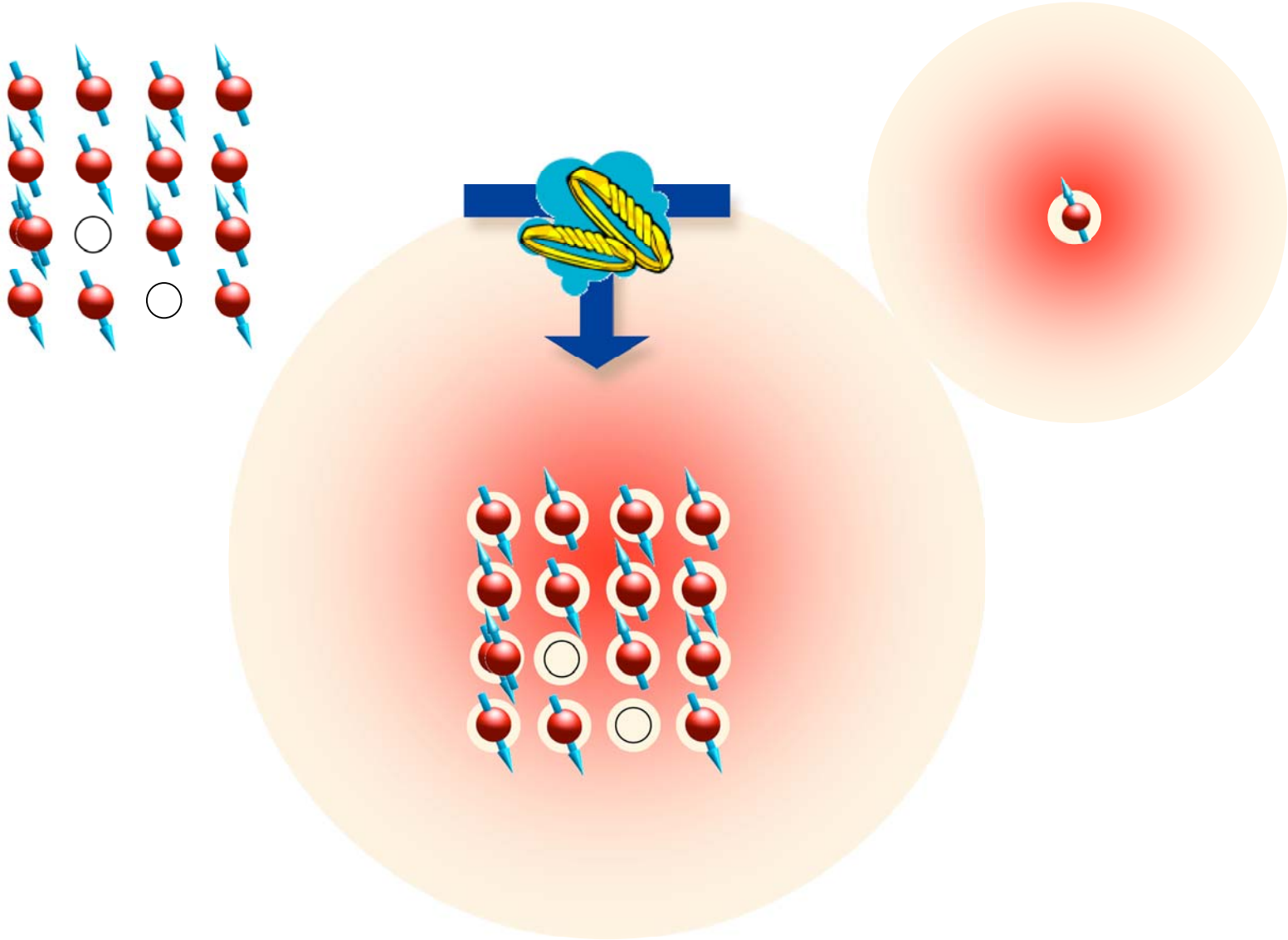
✓ **Exact solution for $N \approx 50$**

- **Mean-field approach**



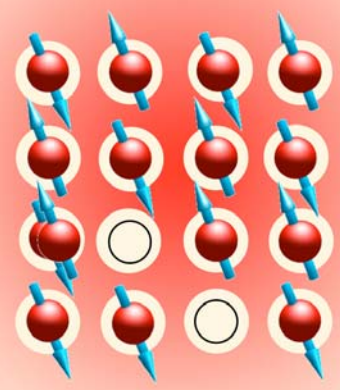
✓ **Thermodynamic limit ($N = \infty$)**

Dynamical Cluster Approximation



Dynamical Cluster Approximation

$$G_0(K,\omega) = \left[\left(\frac{N_c}{N}\sum_{\tilde{k}} \frac{1}{\omega+\mu-\varepsilon_{K+\tilde{k}}-\Sigma_c(K,\omega)}\right)^{-1} + \Sigma_c(K,\omega)\right]^{-1}$$



$$\text{QMC} \rightarrow \Sigma_c[G_0(K,\omega),U]$$

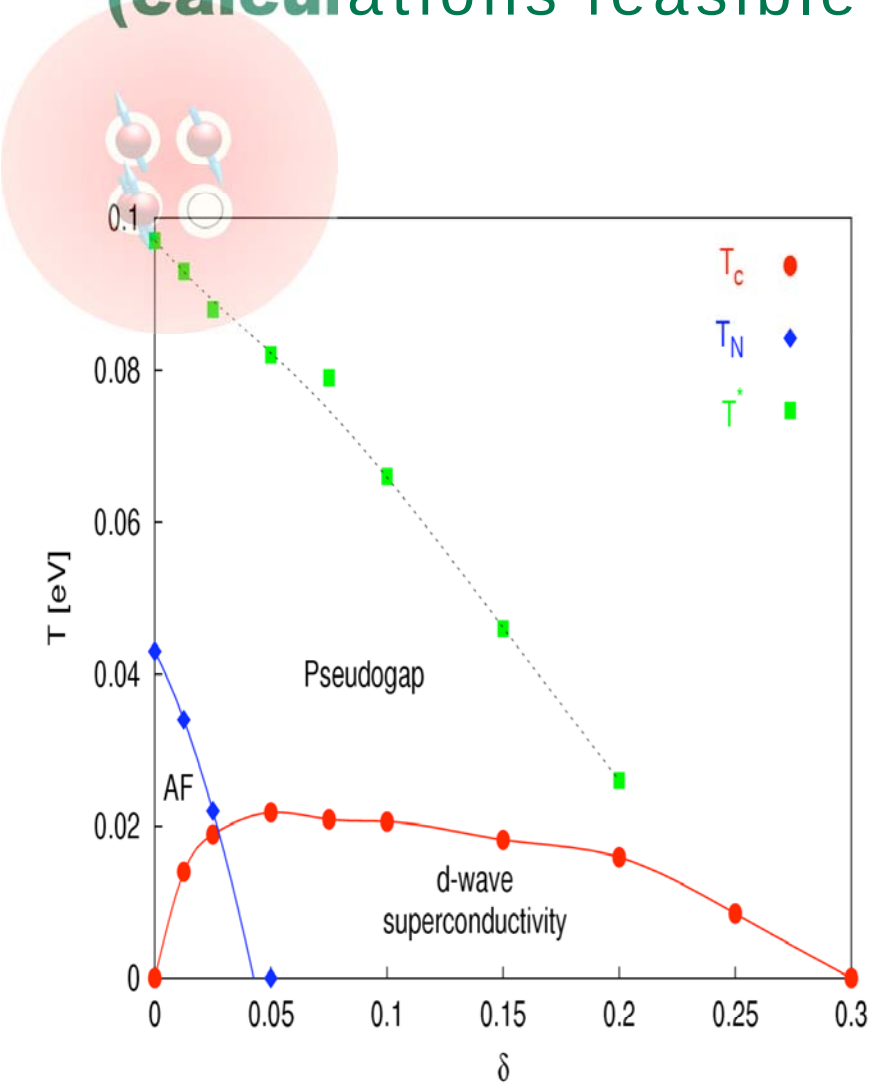
- ✓ **Thermodynamic limit**
- ✓ **Non-local correlations**

Cluster in reciprocal space

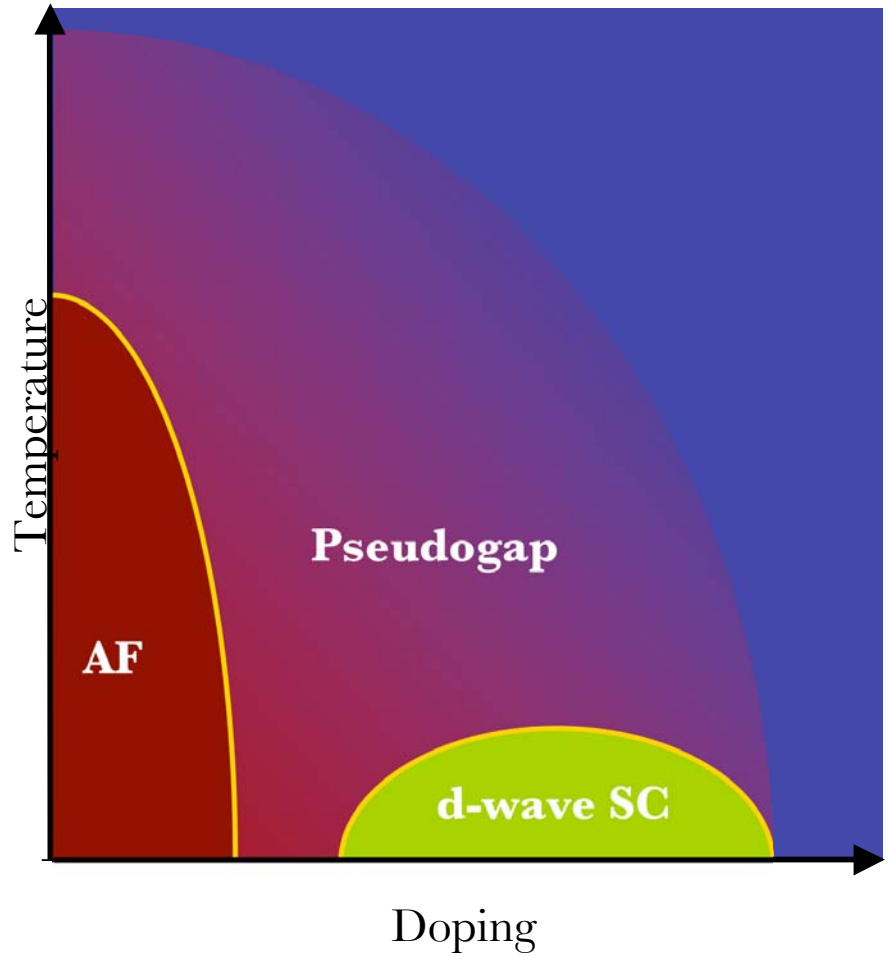
↓

- ✓ **Translational symmetry**
- ✓ **Green's function is causal**

4-site cluster with Quantum Monte Carlo
(calculations feasible on IBM power 4 or Compaq)



Generic HTSC Phase diagram

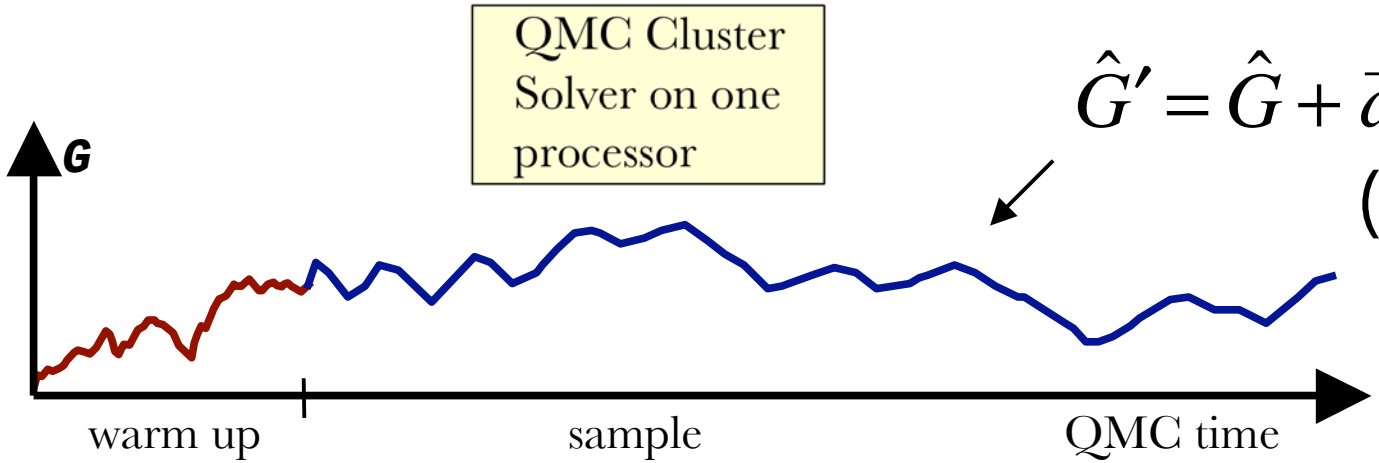


Problem ...

- N_c=4 results in contradiction with Mermin-Wagner theorem:
  - *No finite temperature transition in 2D systems to state with broken continuous symmetry.*
- Consequences:
  - $T_N = 0$
  - Superconductivity only possible as Kosterlitz-Thouless topological order
- Violation caused by small cluster
- Cure: Simulate larger clusters
  - Computational cost grows like $\sim N_c^3$
  - Efficiency breaks down on superscalar machines

DCA/QMC Cluster solver

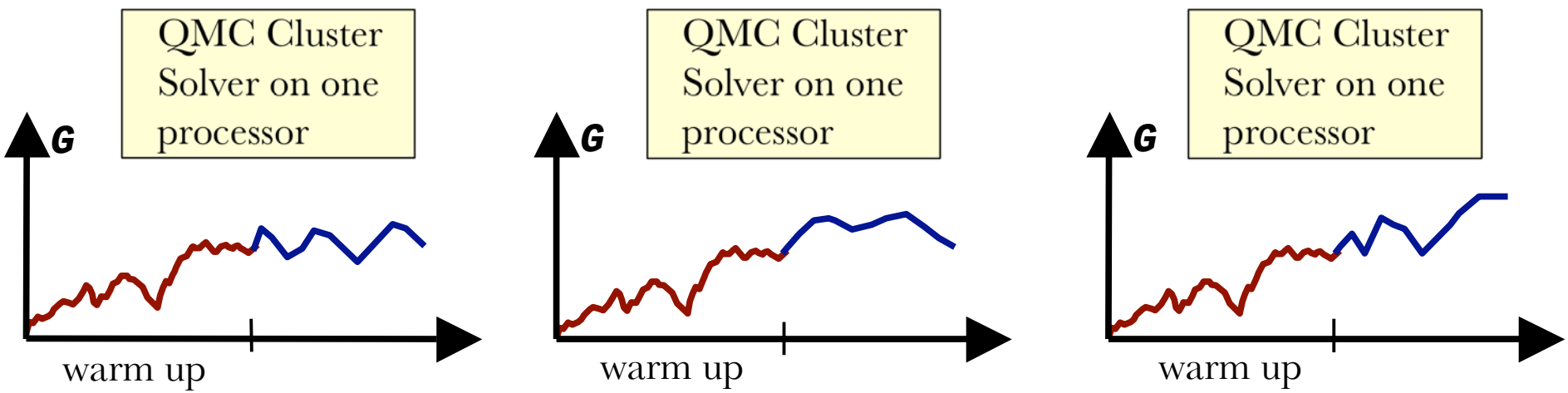
Serial:



$$\hat{G}' = \hat{G} + \vec{a} \otimes \vec{b}$$

(dger)

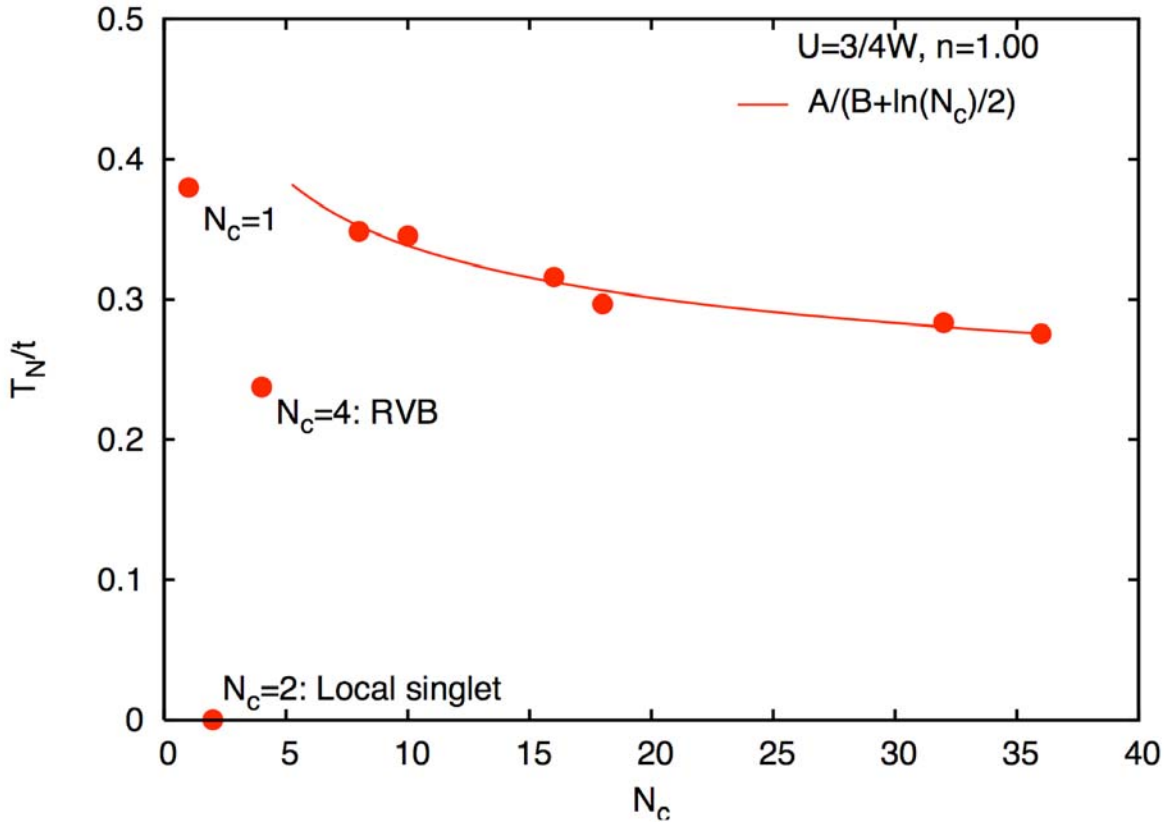
Perfectly parallel:



Performance

- **Quantum Monte Carlo**
  - **Highly parallel, easy to scale, right?**
  - **No, each process has a significant fixed startup**
  - **Favors fewer, faster processors**
- **Dominated by N^3 operations**
  - **CGEMM - level 3 BLAS, easy on memory**
  - **DGER - level 2 BLAS, needs memory bandwidth**
  - **O(1) CGEMMs and O(N) DGERs per step**
  - **DGERs dominate**

Antiferromagnetic transition in 2D Hubbard Model

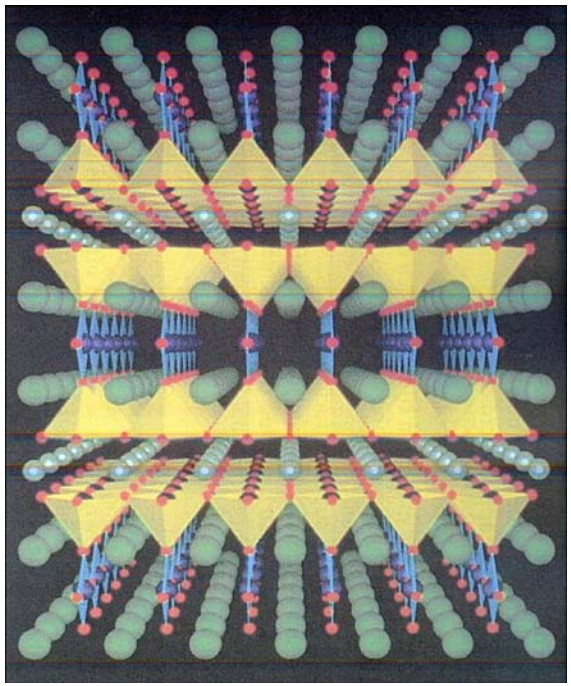


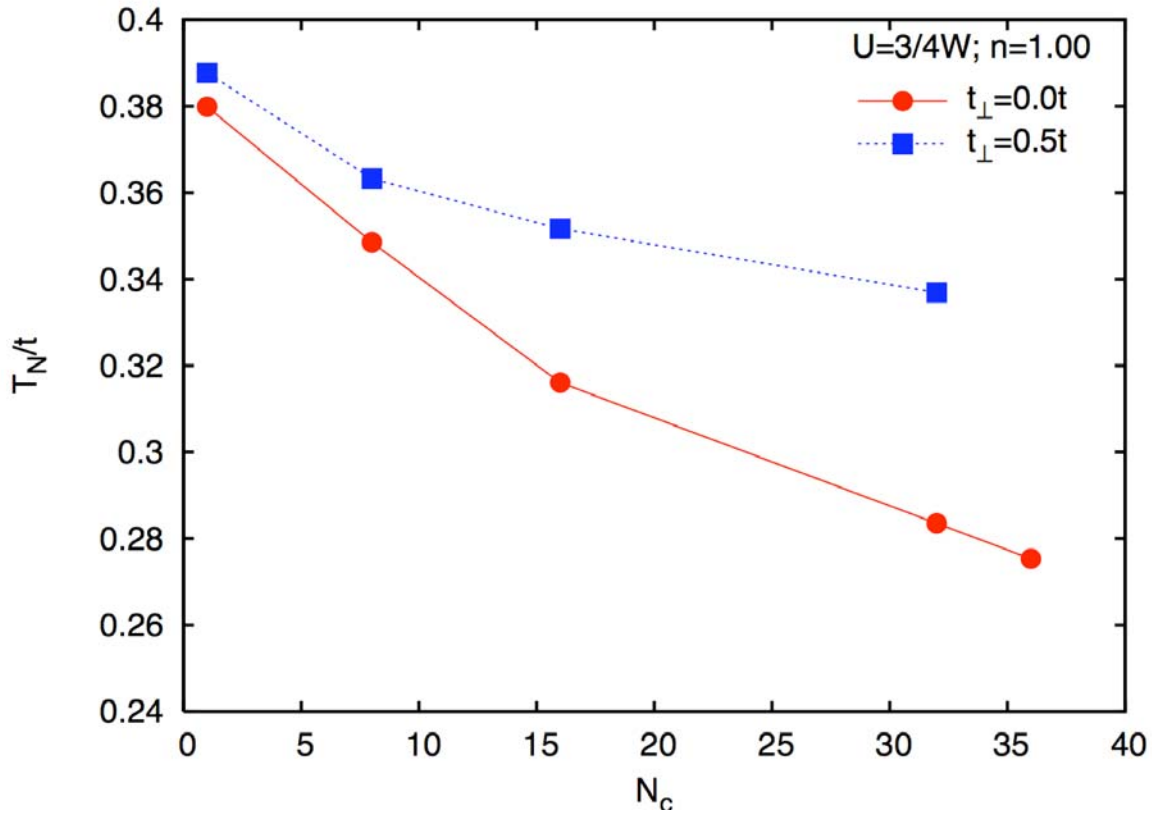
Transition temperature falls logarithmically with cluster size

→ Mermin-Wanger theorem recovered in large cluster limit

Antiferromagnetic transition in real three dimensional crystal

- **Introduce coupling between CuO planes:** $t_\perp$

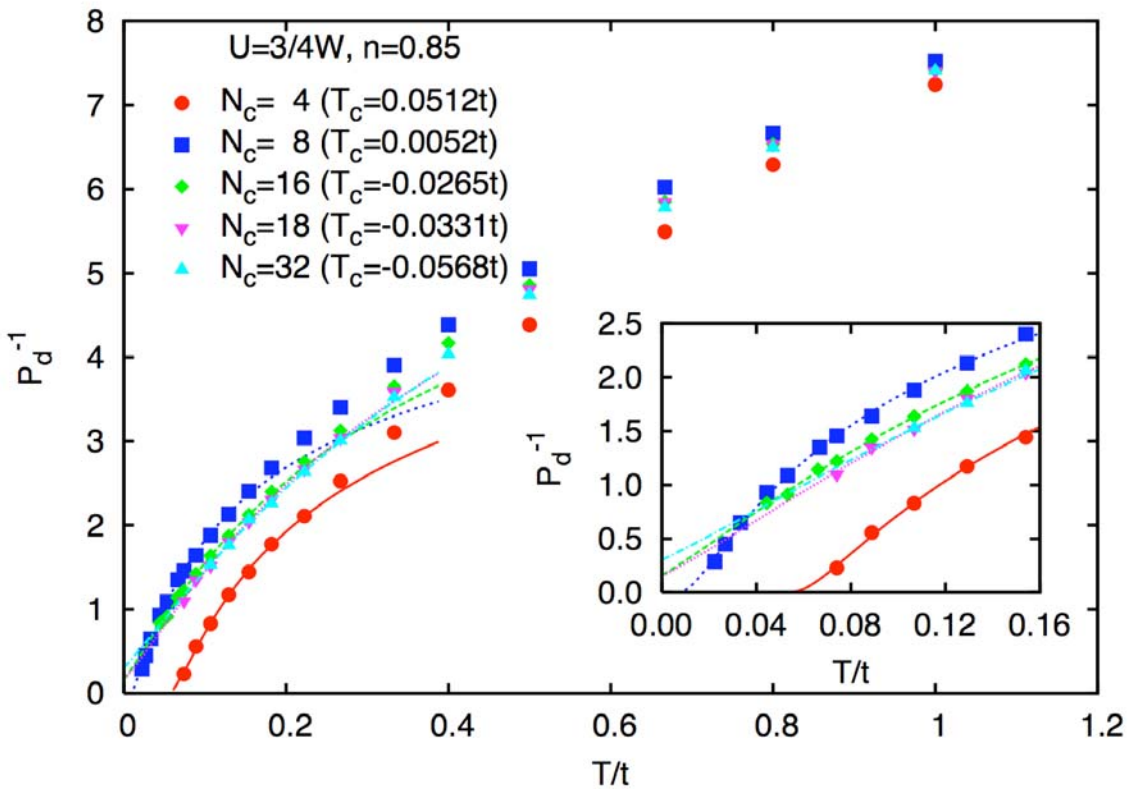




3D crystal has non-zero AF-transition temperature

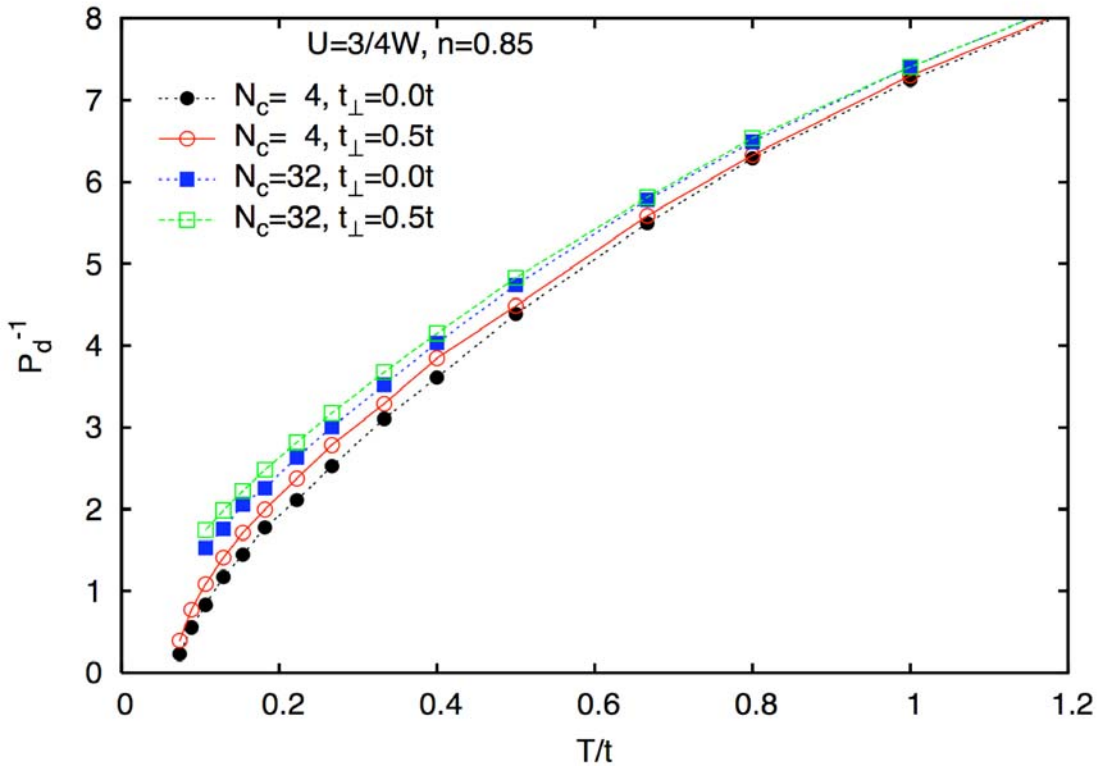
Superconducting Transition

- **Measure pair-field susceptibility: diverge?**



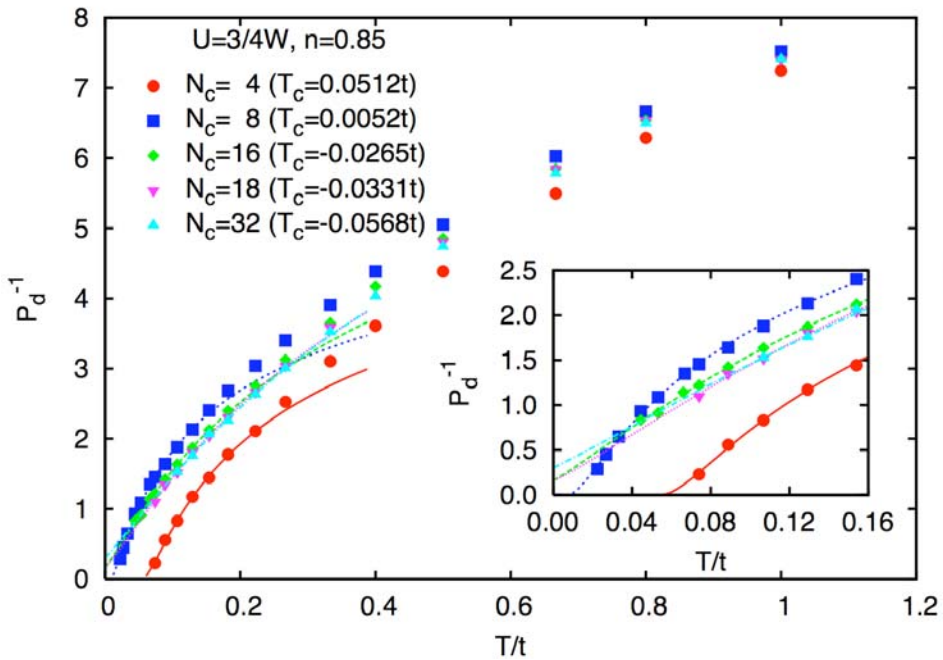
A SC transition appears to be missing!

With inter-planar coupling (introduced as perturbation)



3D coupling seems to further inhibit transition

Can we reach lower temperatures: The $1M Question



- **Need to reach lower temperatures for large cluster**
- **Sign problem of QMC:**
  - **Number of needed measurements grows exponentially**

$$M \sim \exp(2\beta U L_c)$$

- **Sign problem is *NP*-hard (Troyer and Wiese 2004):**
  - **Solving it means solving one of the millennium challenges**
  - **Winn $1M (www.claymath.org) and possibly a Nobel Prize**
- **Our current plans are less ambitious: reduce *U*~1/2*W***
  - **Ongoing calculations, results expected by end of calendar year**

Summary / Conclusions

- **High temperature superconductivity:**
  - **Pairing mechanism still a mystery**
- **Computational Challenge:**
  - **Solve a macroscopic quantum problem (N~10^{23})**
  - **Account for non-local correlations at nano-scale**
- **Dynamical Cluster Approximation**
  - **Self-consistently embed clusters in effective medium**
  - **Recover exact solution as N_c reaches system size**
- **DCA/QMC on Cray X1**
  - **Reach cluster sizes that capture relevant physics**
  - **Properly describe antiferromagnetism of Cuprates superconductors**
- **Microscopic solution of high temperature superconductivity problem within reach!**

Acknowledgments

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