Simulations of correlated electrons: What's under the superconducting dome in the two-dimensional Hubbard model?

Mark Jarrell

CMSN

PIRE DMR

Outline

- Modeling the Cuprates
- Methods
- What's under the dome?
  - Quantum Criticality
  - Evidence for QCP
  - Nature of the QCP
- Challenges and Future

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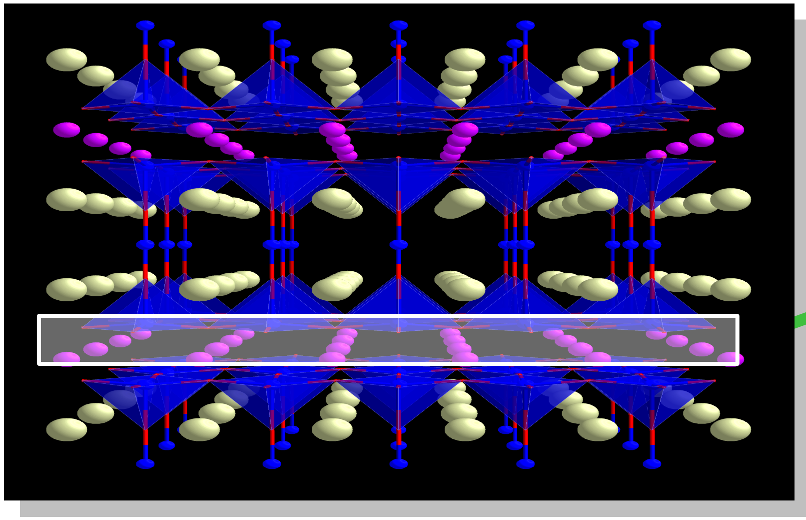
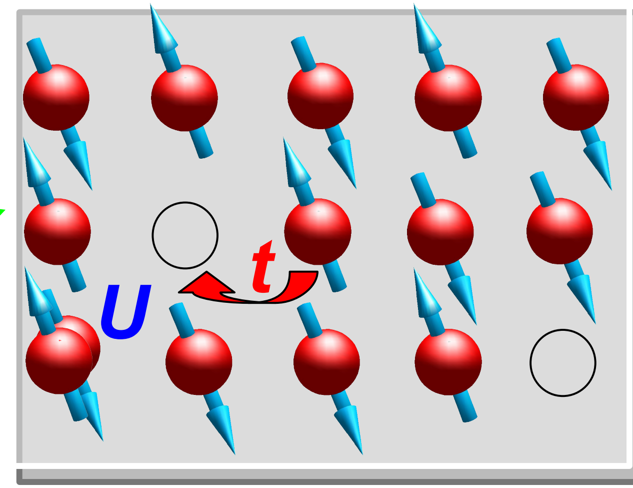
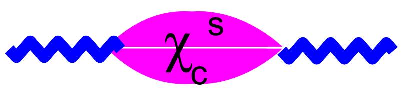
Modelling The Cuprates





- Pairing driven by AF spin fluctuations



- Doped Mott+AF insulator
- Model due to Anderson and ZR
- Model from downfolding LDA (NMTO)

(Zhang and Rice, PRB 1988, P.W. Anderson)

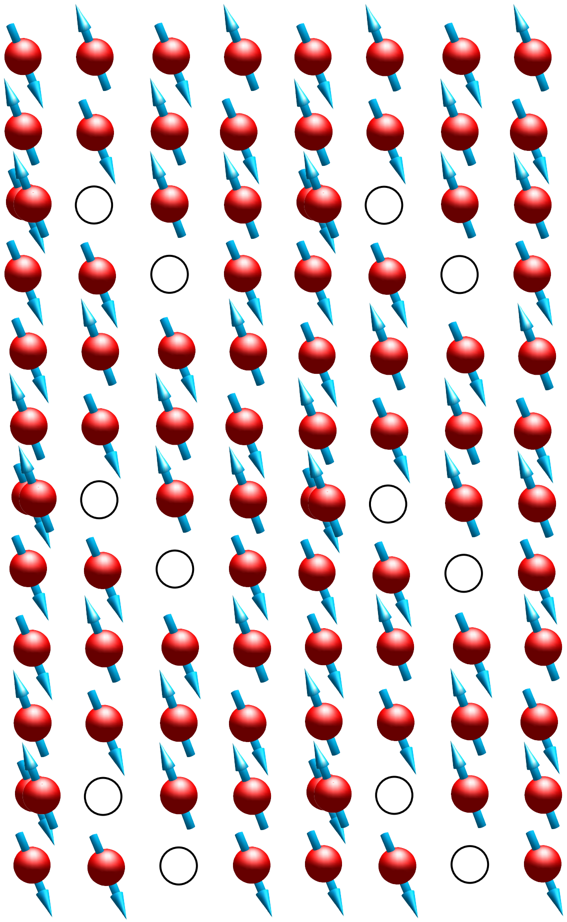
$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

U/W<<1 Bickers, PRL 1989; Monthoux, PRL 1991; Scalapino, JLTP 1999

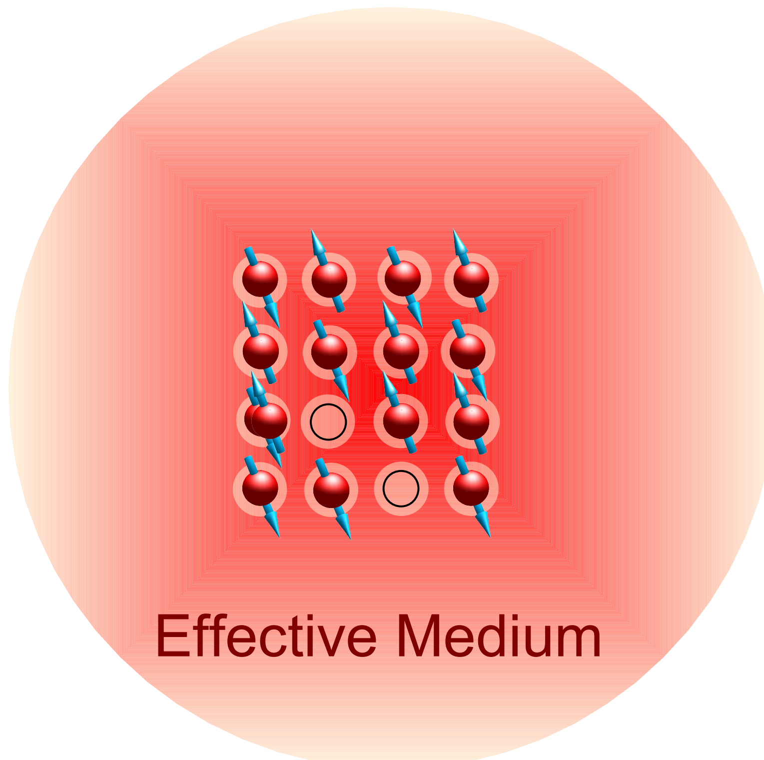
U/W>>1 Sorella, PRL 2002h

Dynamical Cluster Approximation

Periodic Lattice



DCA

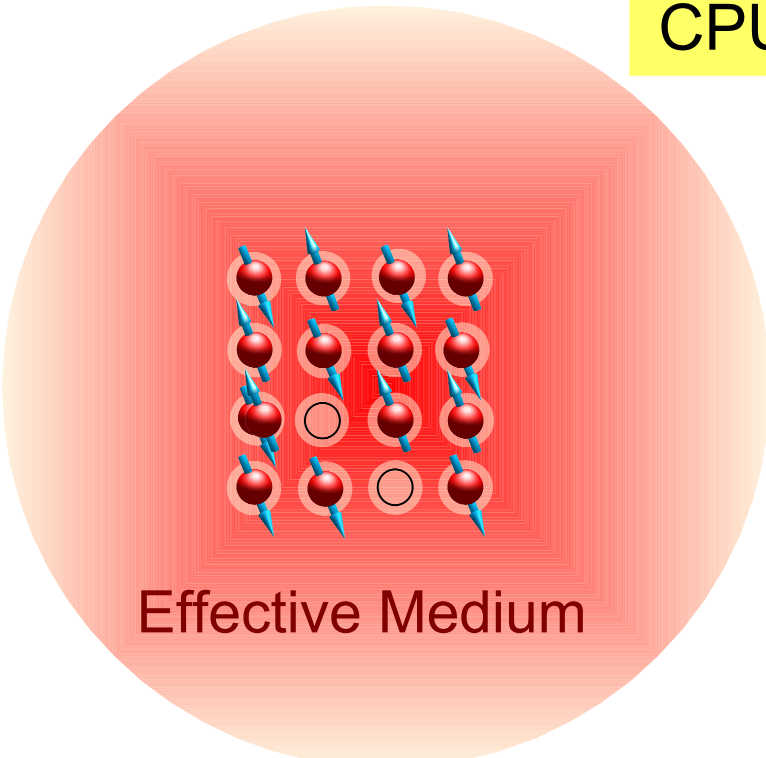


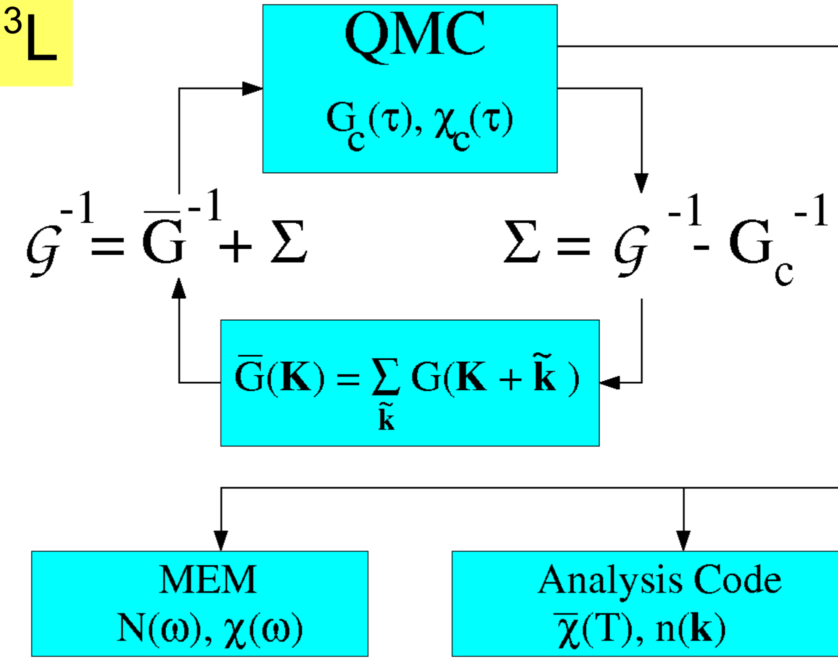
- Short length scales, within the cluster, treated explicitly.
- Long length scales treated within a mean field.
- N_c=1 DMF, $N_c=\infty$, exact

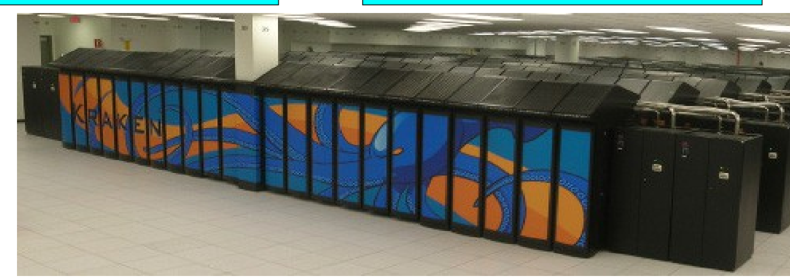
For a review of quantum cluster approaches: Th. Maier *et al., Rev. Mod. Phys. 77, pp. 1027 (2005).*

Quantum Monte Carlo (QMC) Cluster Solver

CPU ~ N^3L





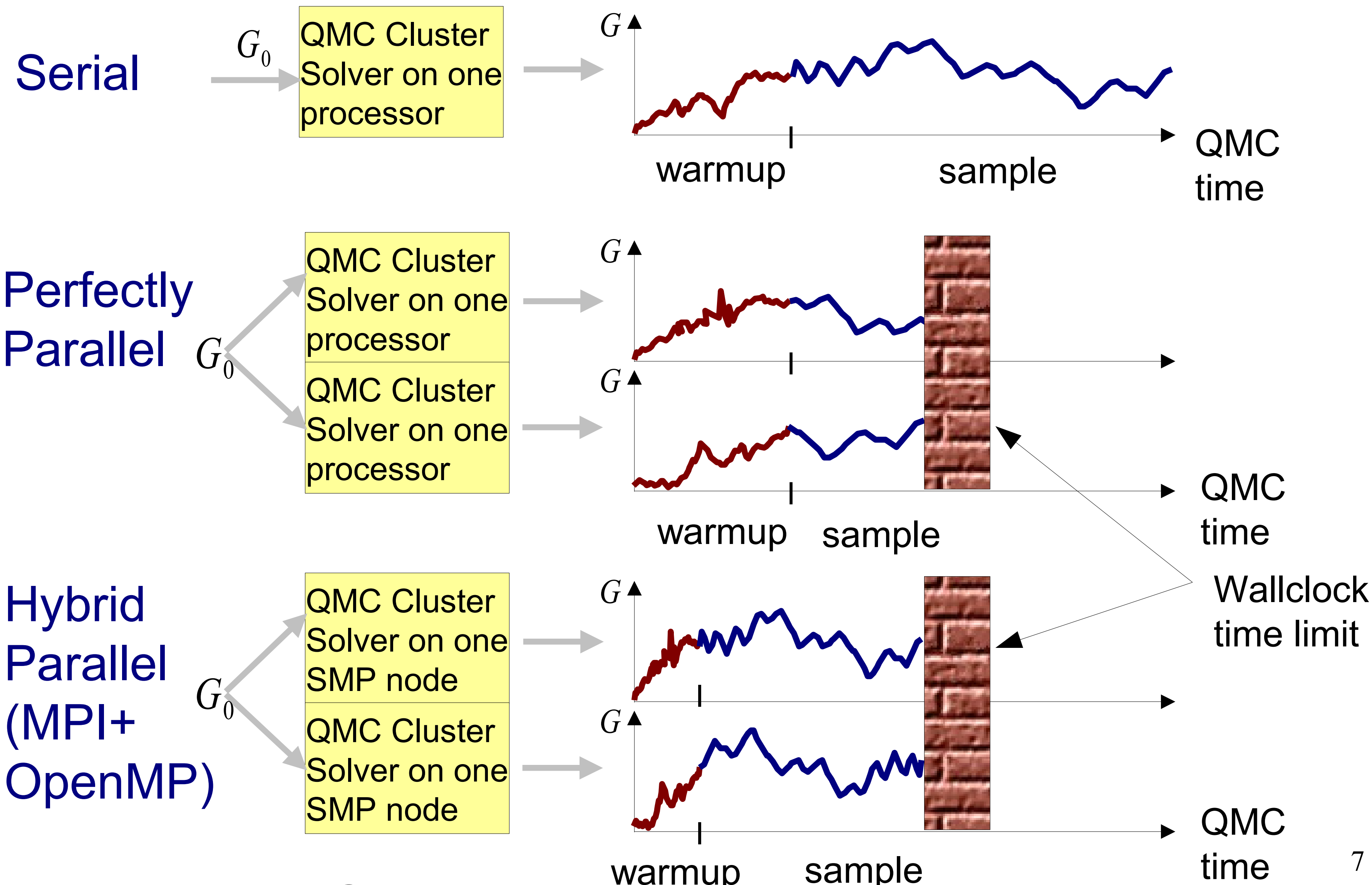


- A QMC Algorithm for Non-local Corrections to the Dynamical
- Mean-Field Approximation, M. Jarrell, PRB 64, 195130/1-23 (2001)
- A. N. Rubtsov, et al., Phys. Rev. B 72, 035122 (2005).
- ArXiv:0904.1239 Dynamical Mean Field Theory Cluster Solver with **Linear Scaling in Inverse Temperature**, E. Khatami, et al.

02/09/10

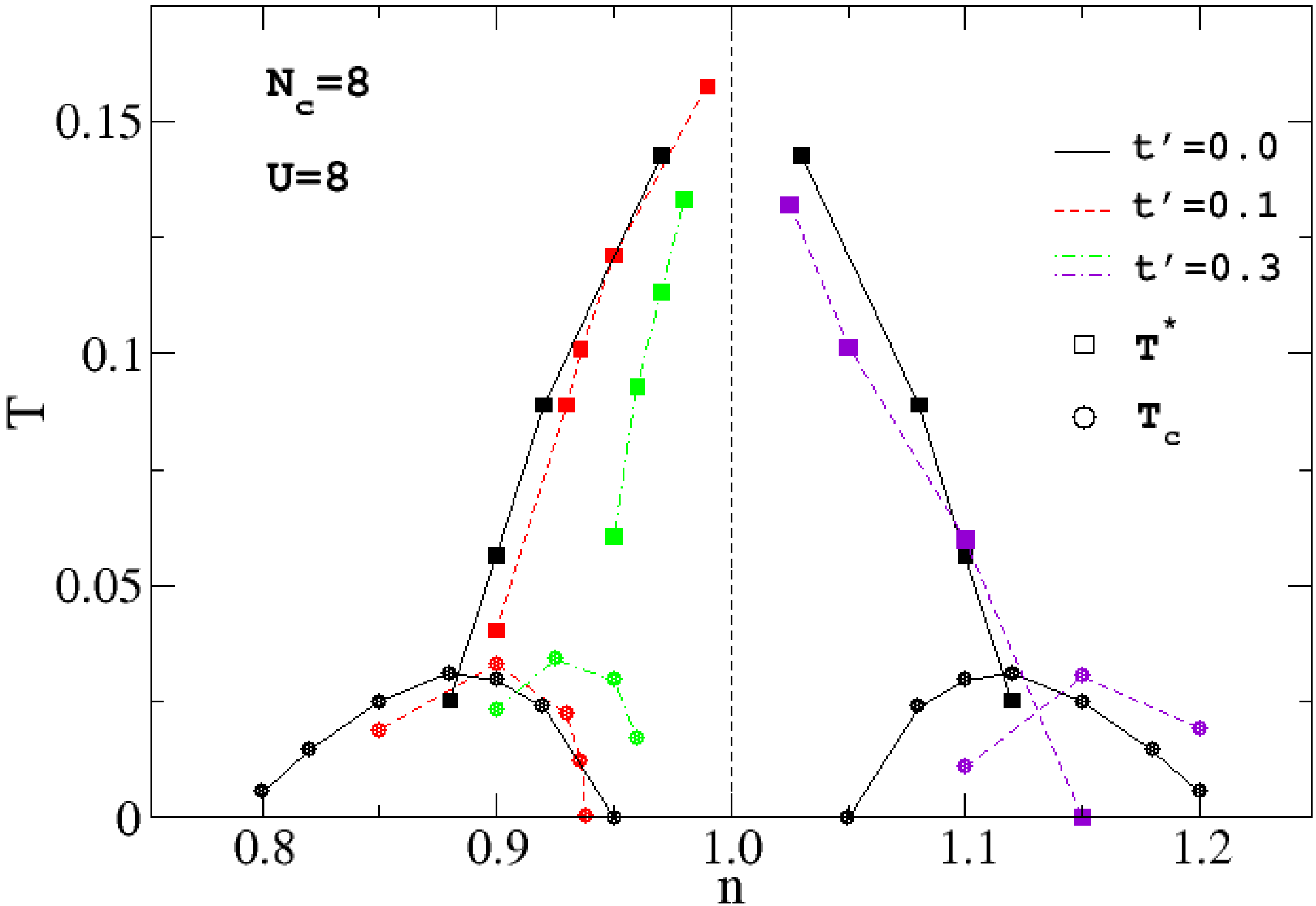
Jaguar or Kraken XT5

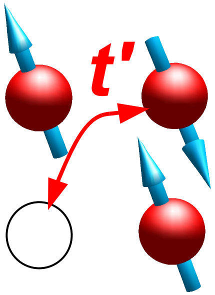
Parallelization of QMC Cluster Solver

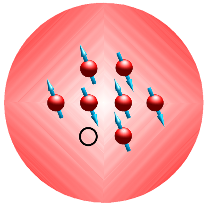


All inner loops GEMM

Superconducting phase diagram







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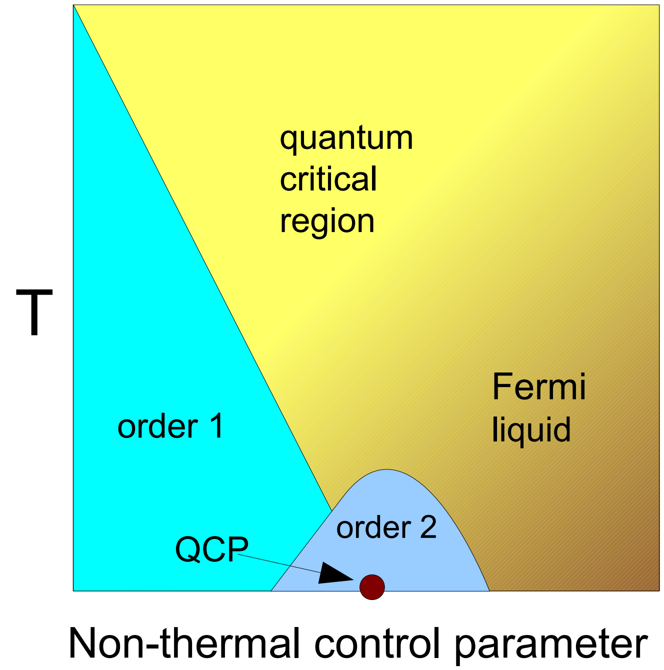
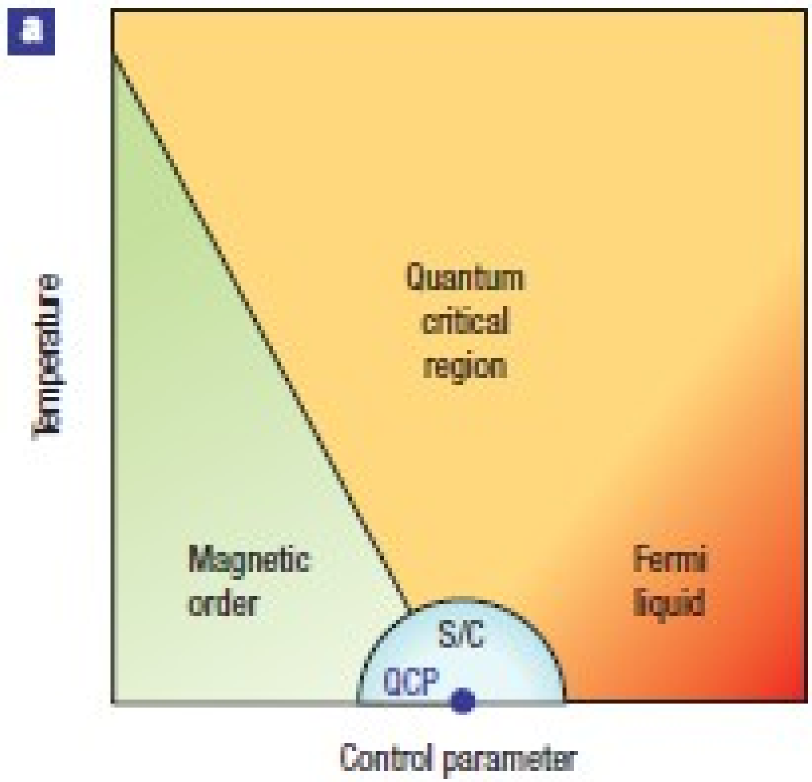
Quantum Criticality

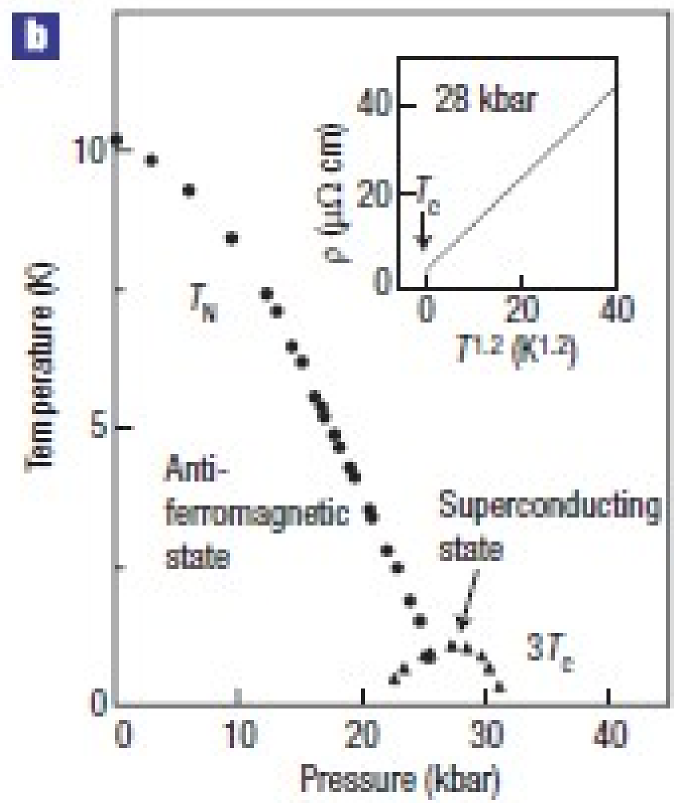


- QCP where Tc of order 1 vanishes
    - No entropy, order-to-order transition driven by energy
    - Heisenberg fluctuations, no thermal fluctuations
    - Effects a very wide range of temperatures
- A second order, driven by remnant fluctuations, often emerges near the QCP

Quantum Criticality In Heavy Fermion Systems

$CePd_2Si_2$

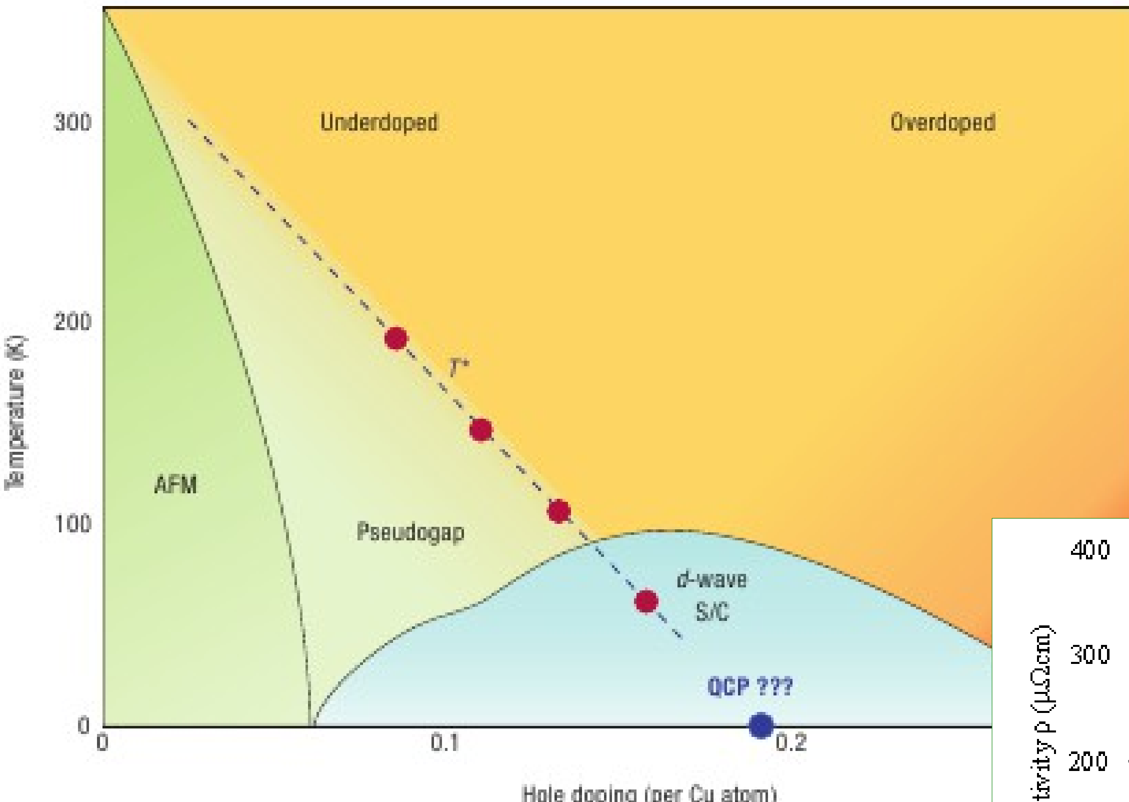




D.M. Broun, Nature Physics, 4, 170

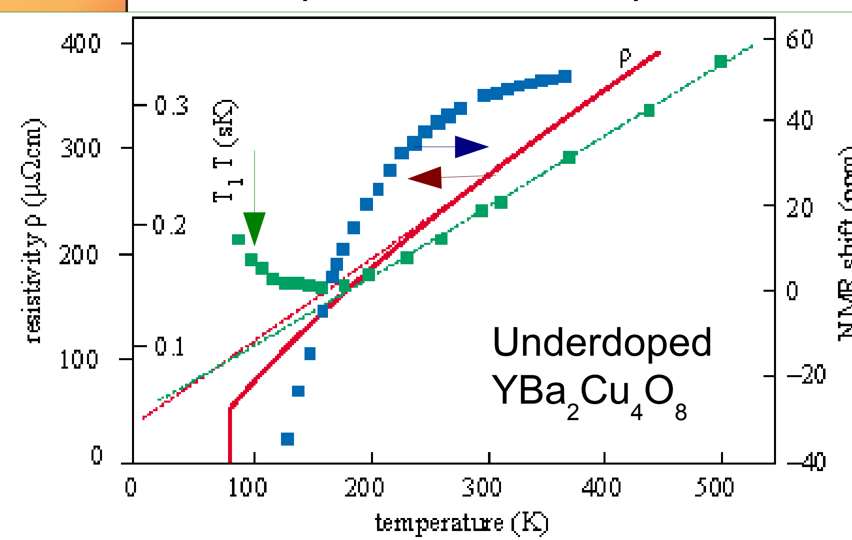
N. Mathur, Nature, 394, 41

Quantum Criticality In The Cuprates



D.M. Broun, Nature Physics, 4, 170

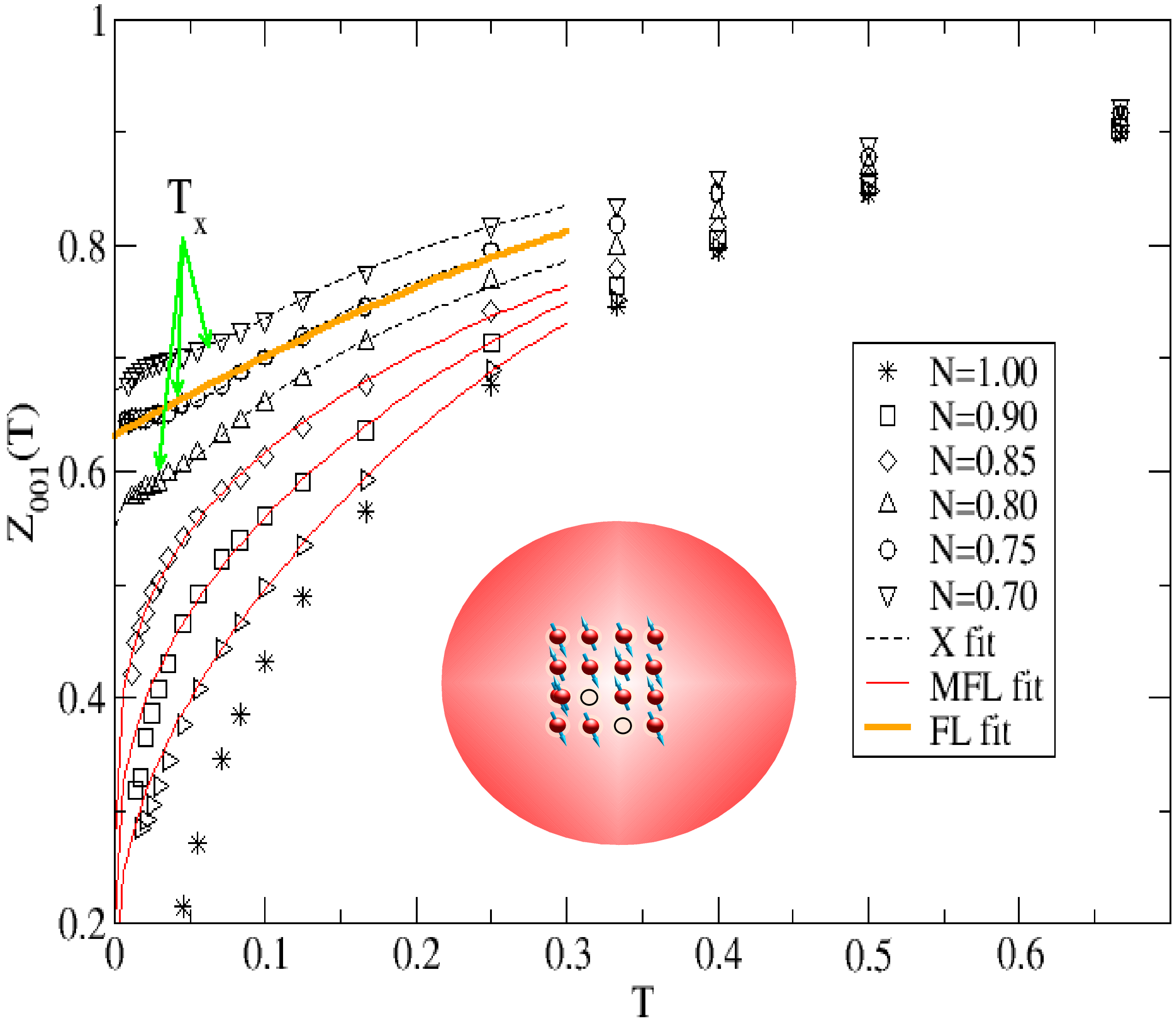
- QCP seen in
  - Resistivity
  - NMR
  - C
  - Kerr effect
  - Neutrons
- No obvious vanishing transition temperature or order parameter

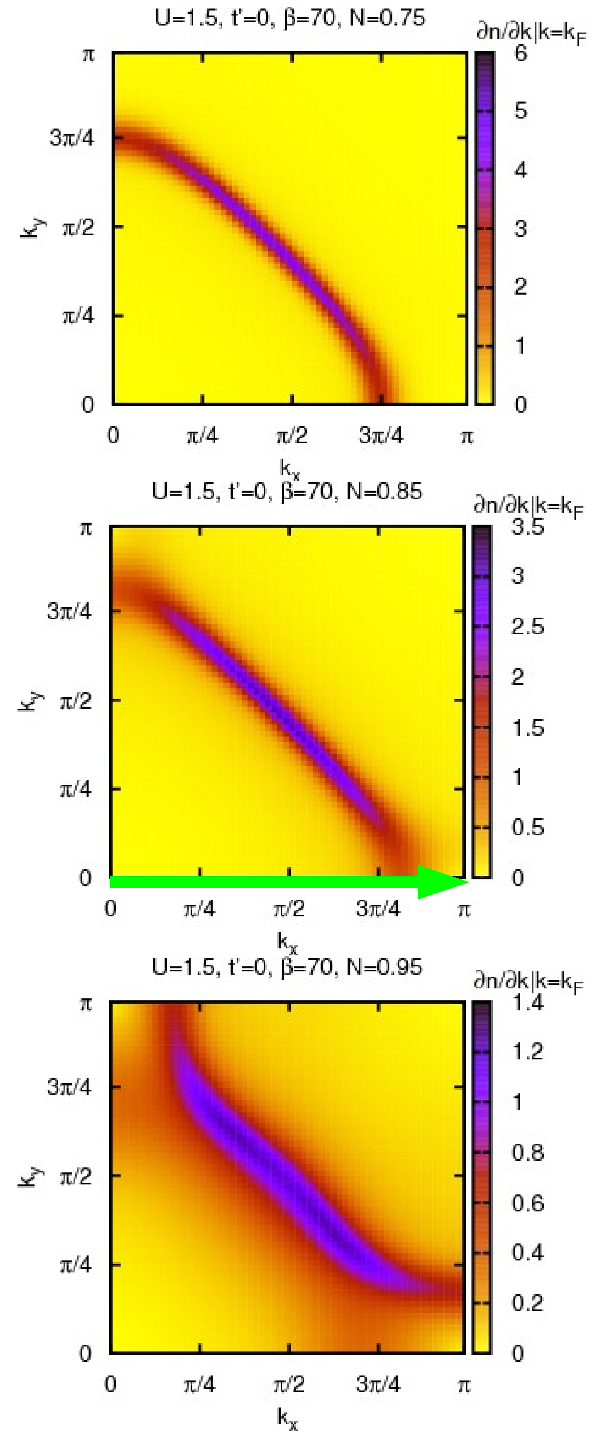


$$\Sigma''(\omega) \approx -\alpha\, max(|\omega|, T)$$

B. Batlogg and C.M. Varma, Physicsworld, Feb, 01

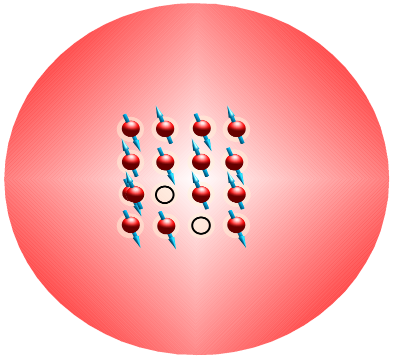
Matsubara QP fraction Z_{001}

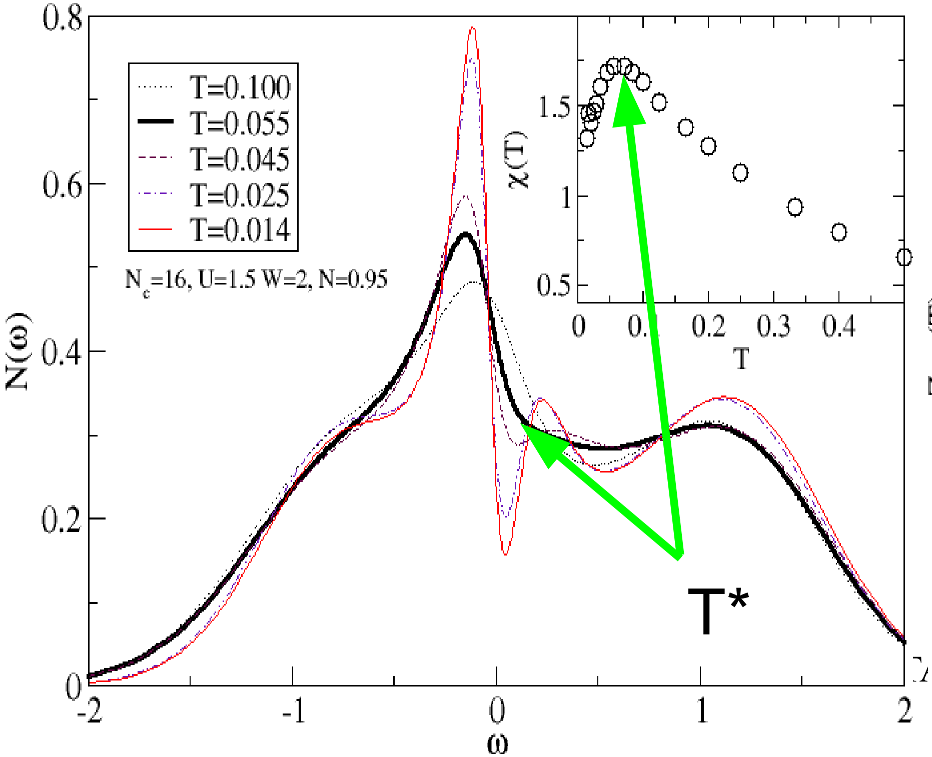


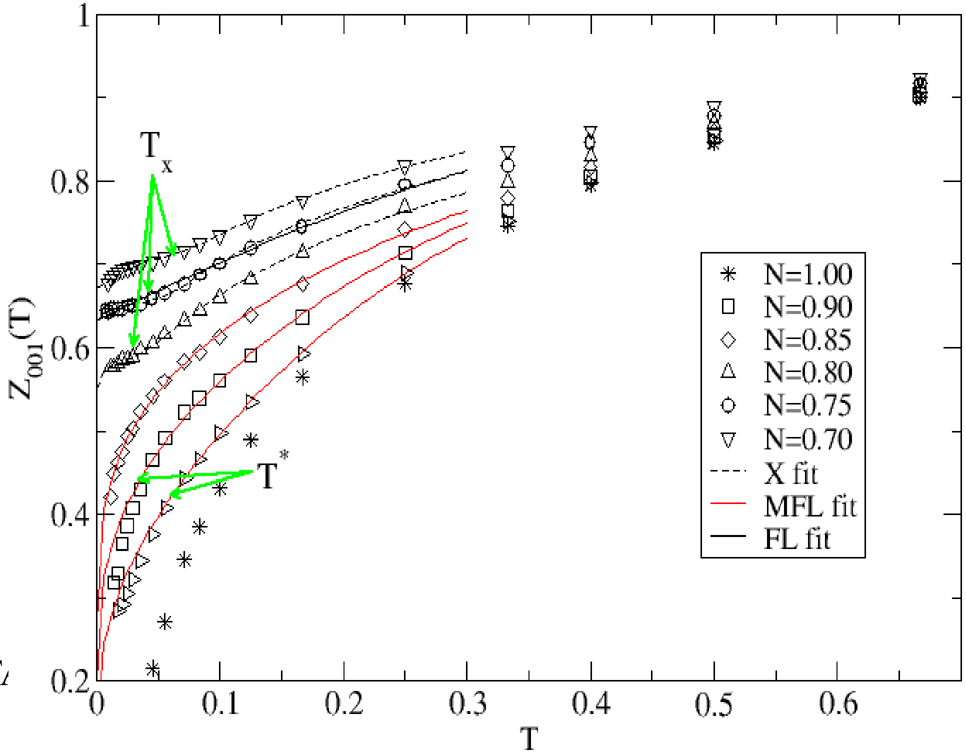


Pseudogap temperature

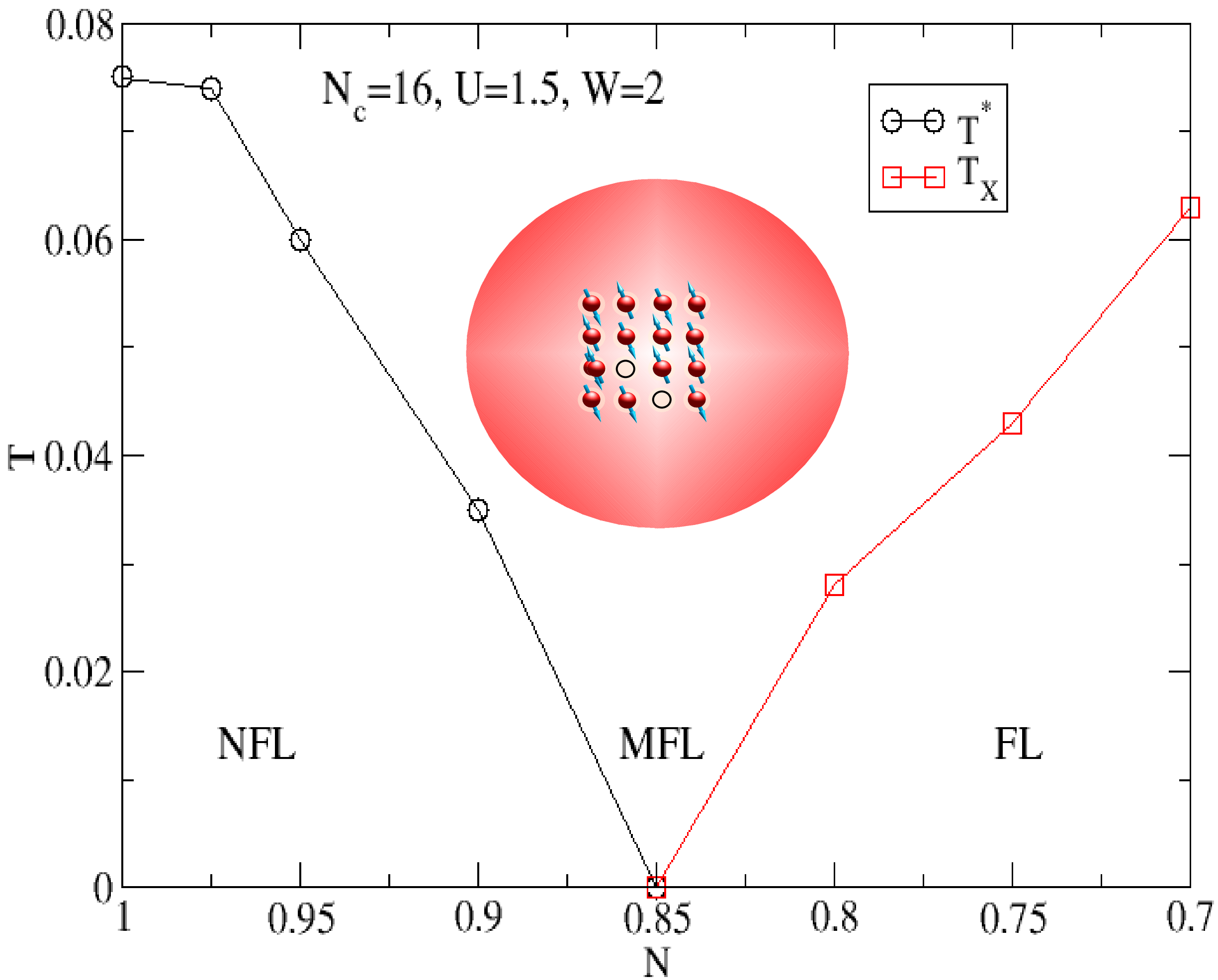
- Pseudogap indicated by a concomitant dip in N(w) and downturn in χ(T) indicating a suppression of S=1 excitations
- Z_{001} (T) shows deviation from MFL for T<T*







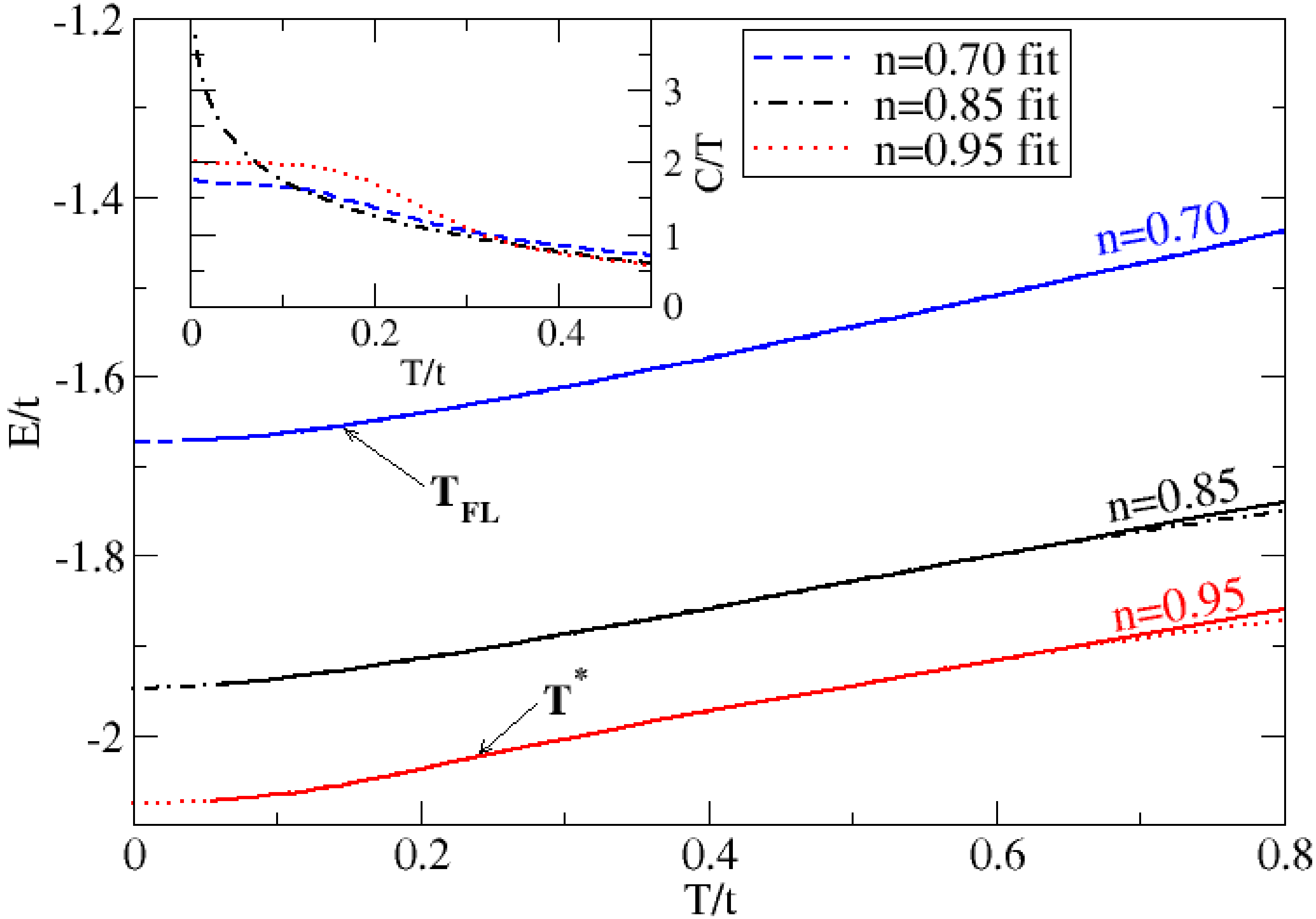
Quantum Critical Phase diagram



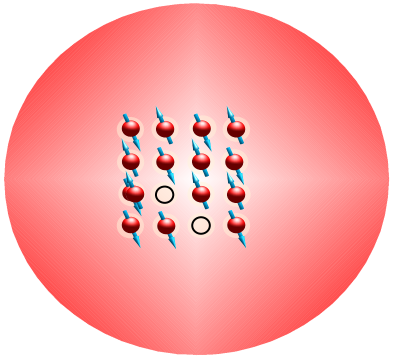
- QCP at finite doping.
- low T NFL → FL crossover with doping*
- MFL above QCP
- Critical N depends on U(~0.22 for U=8t)
- QC behavior for T≤ 2J
- Why QCP?

* FL→FL, no MFL in t-J model: K. Haule, PRB, 2007

Thermodynamics



K. Mikelsons,
PRB to appear
arXiv:0909.0498

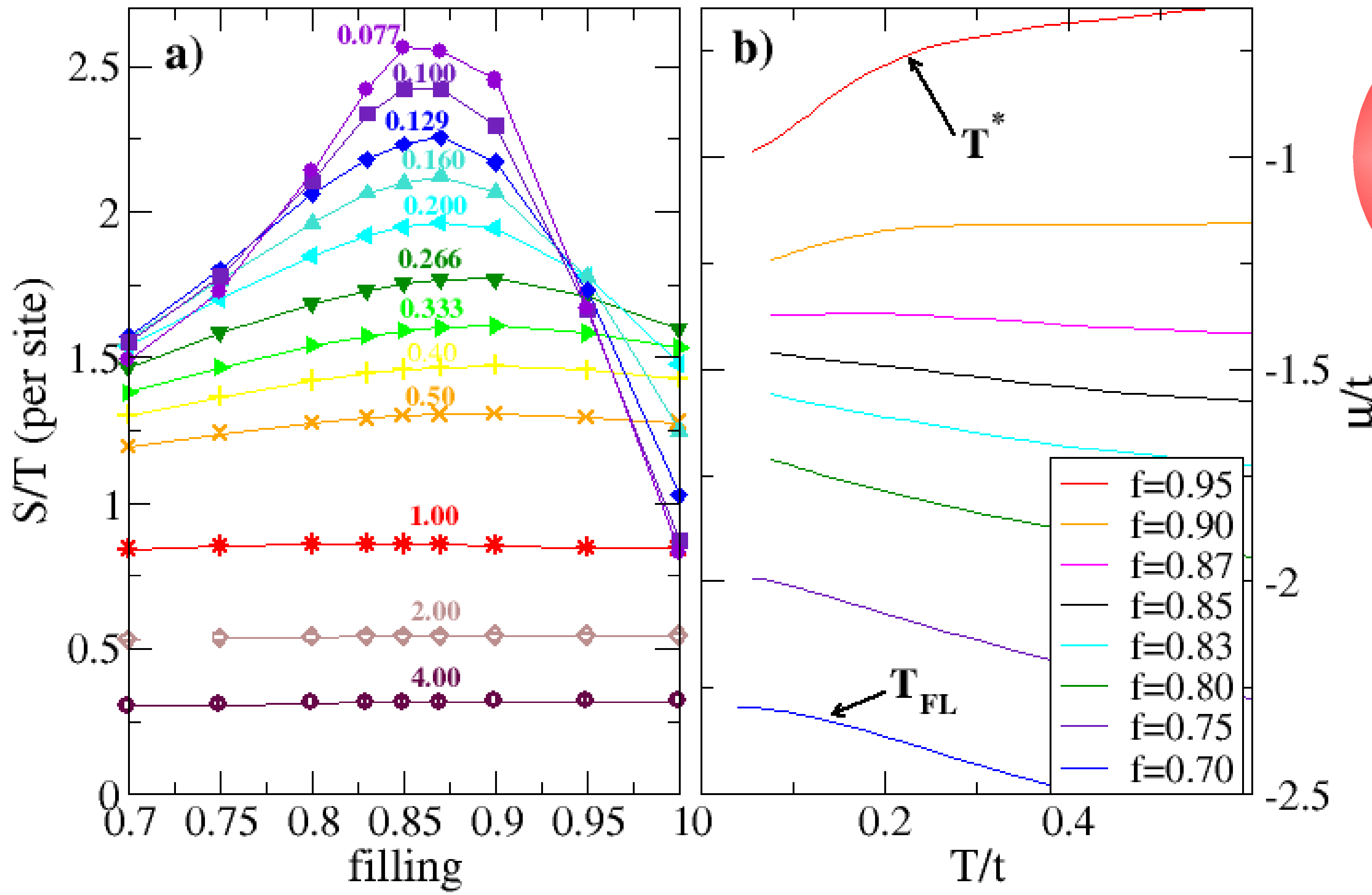


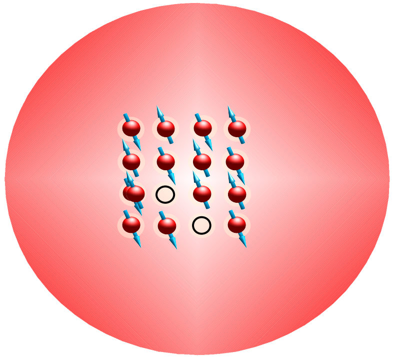
$$E(T) = E(0) + Af(T)T^2 + B\left(1 - f(T)\right)T^2 \ln\left(T/\omega_c\right)$$

Entropy

$$S(\beta, N) = S(0, N) + \beta E(\beta, N) - \int_0^\beta E(\beta', N) d\beta'$$

F. Werner
PRL





$$\left(\frac{\partial S}{\partial N}\right)_{T,U} = \left(\frac{\partial \mu}{\partial T}\right)_{U,N}$$

S/T constant
C~T

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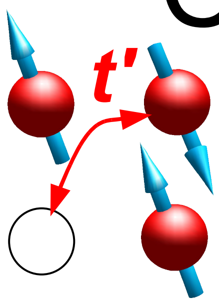
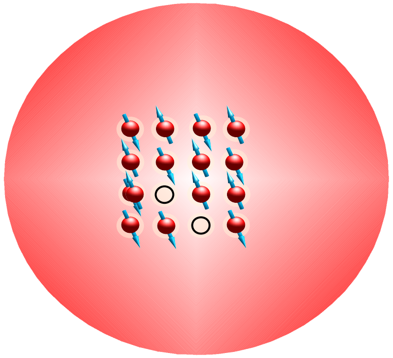
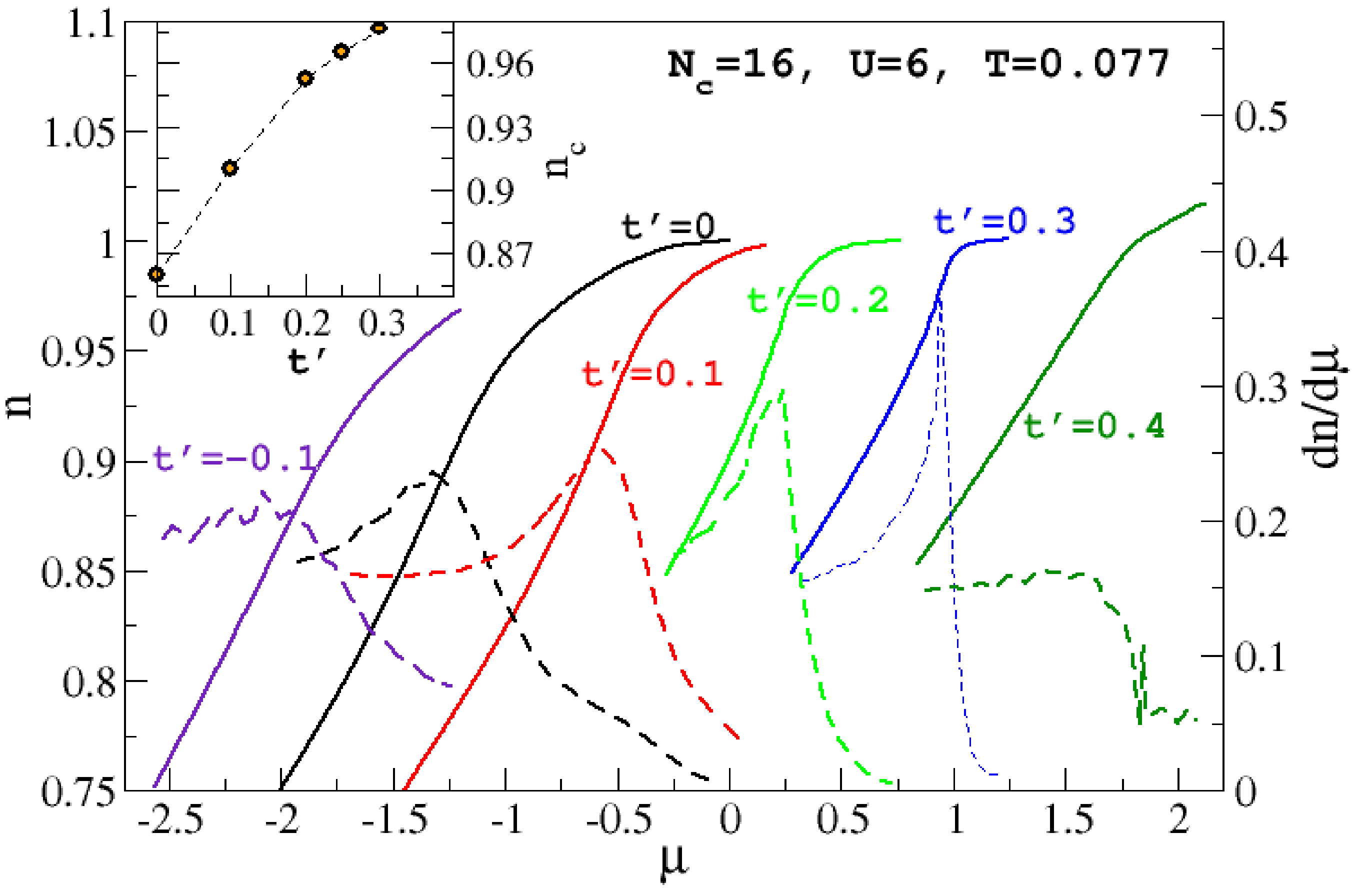
Charge Fluctuations at QCP



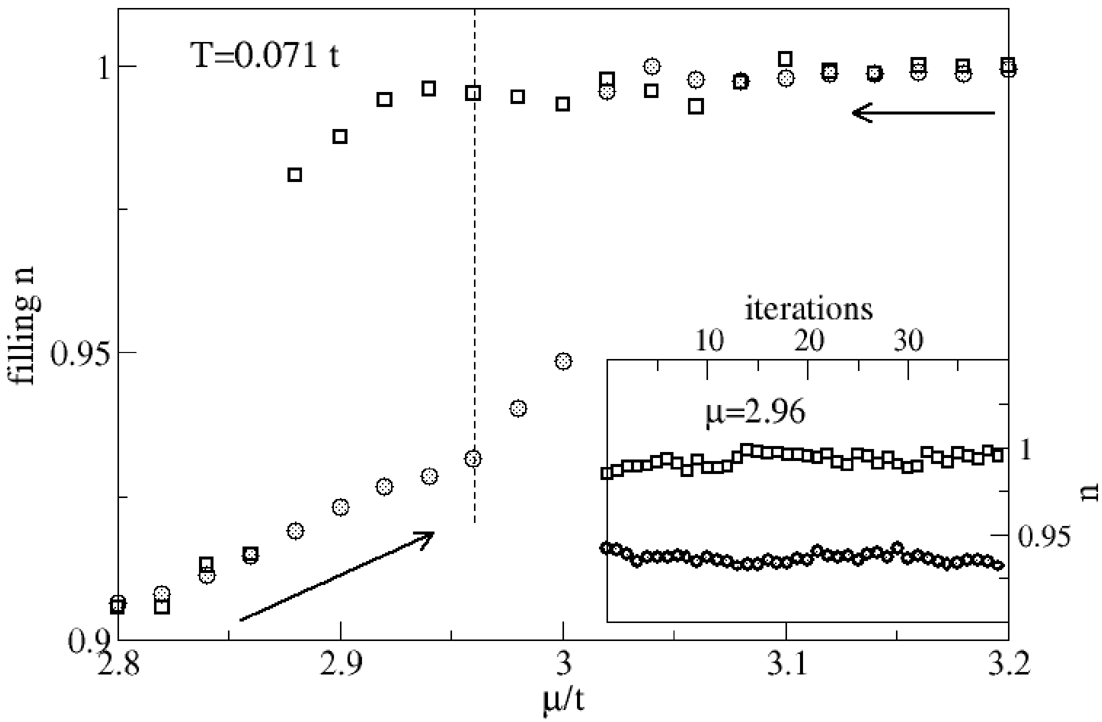




- For t'=0 peak in charge susc. at QC filling
- As t' increases the peak becomes sharper

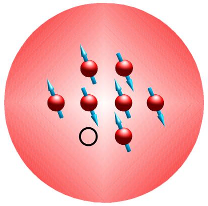
Phase separation at lower T

Repeatable hysteresis

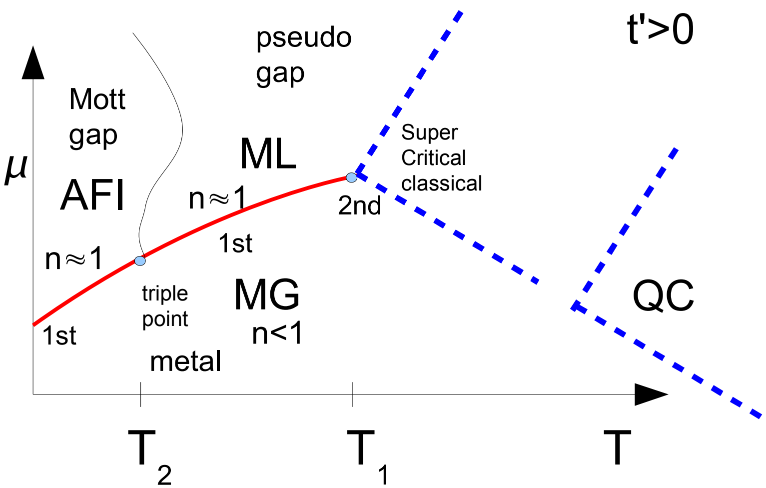


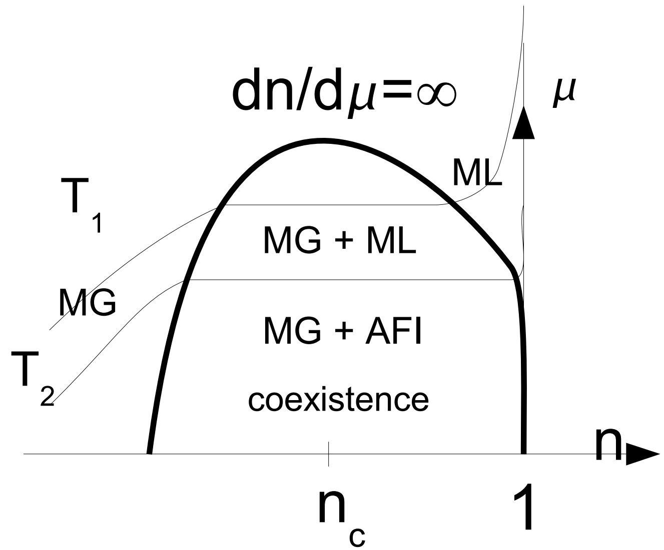
- U/t=8, t'/t=0.3, T=0.071t
- Hysteresis for T<T_c $\approx 0.1t$
- PS at finite T seen only when t'$\neq$ 0
  - G. Su, PRB, 1996
- Two Solutions found
  - Compressible, hole rich (Mott Gas)
  - Incompressible, hole poor (Mott Liquid)

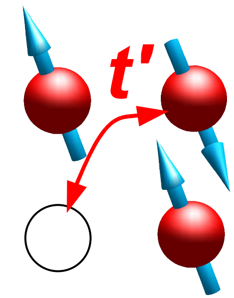
Macridin, PRB (2006)

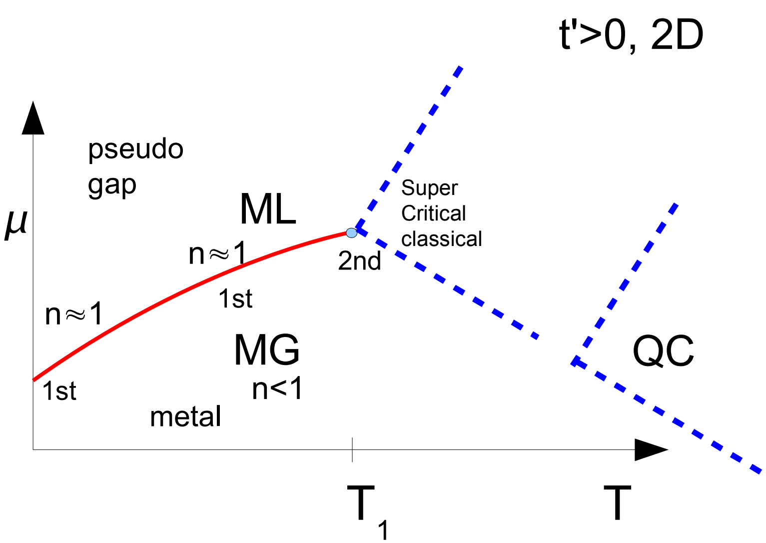


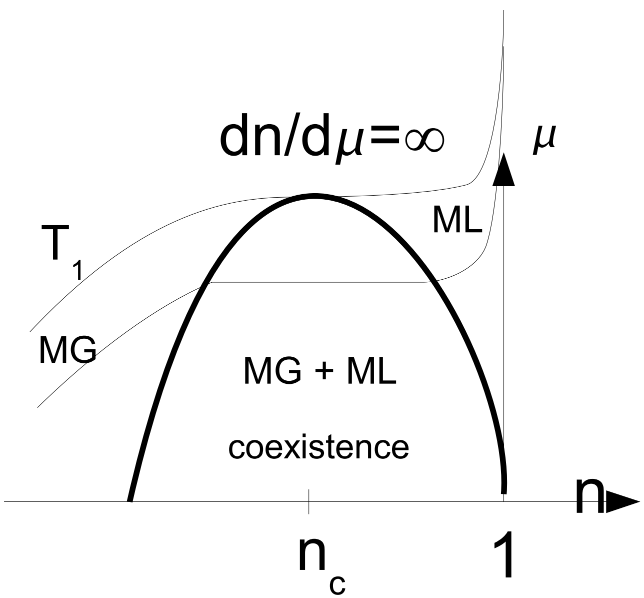
Analogy to Liquid-Gas-Solid phase diagram

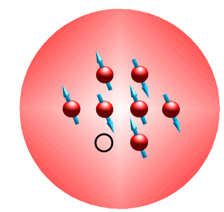




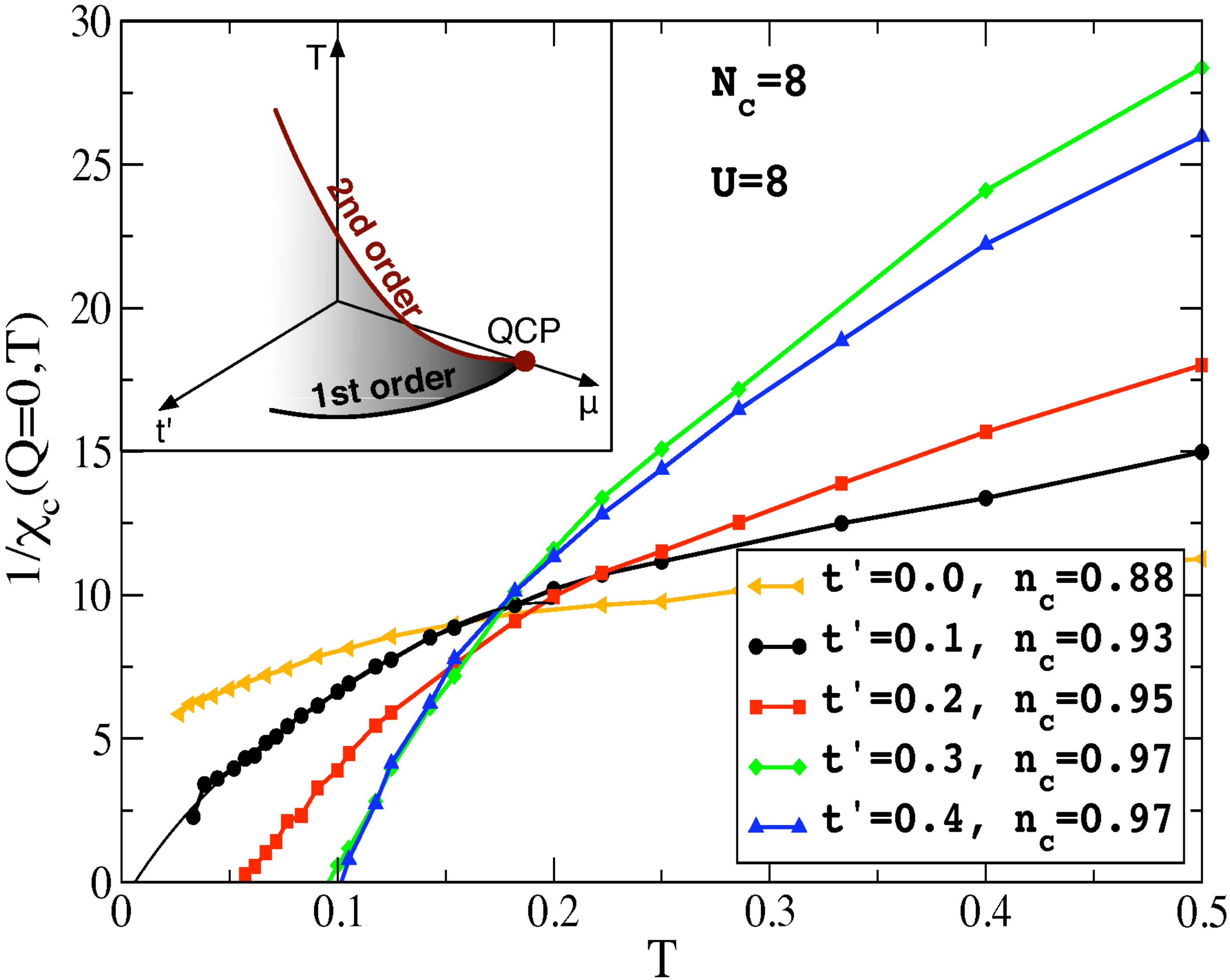


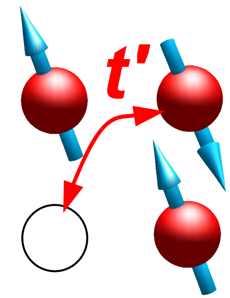


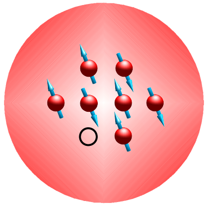




Phase separation diagram

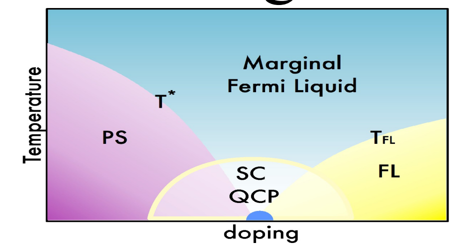




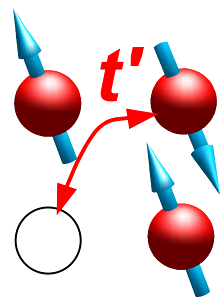


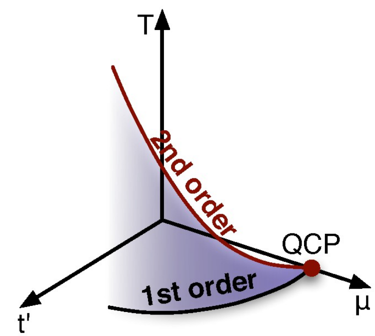
Conclusion

- Superconductivity and QCP are found in the Phase Diagram of the Hubbard Model

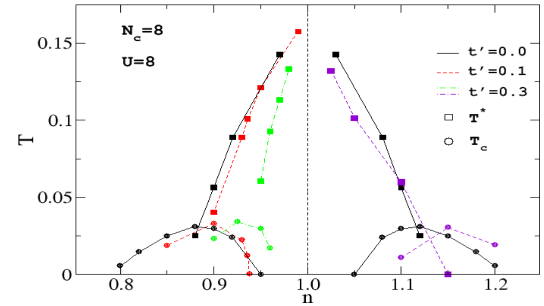


- QCP in the 2D Hubbard Model:
  - Due to a T=0 second order terminus of a line of first-order phase separation transitions.
  - Dependence on t'/t





- Questions:
  - What drives the Phase Separation ?
  - What drives superconductivity at the QCP ?
  - QCP for t'/t < 0 ?
  - Role of phonons (prelim: increase PS)?



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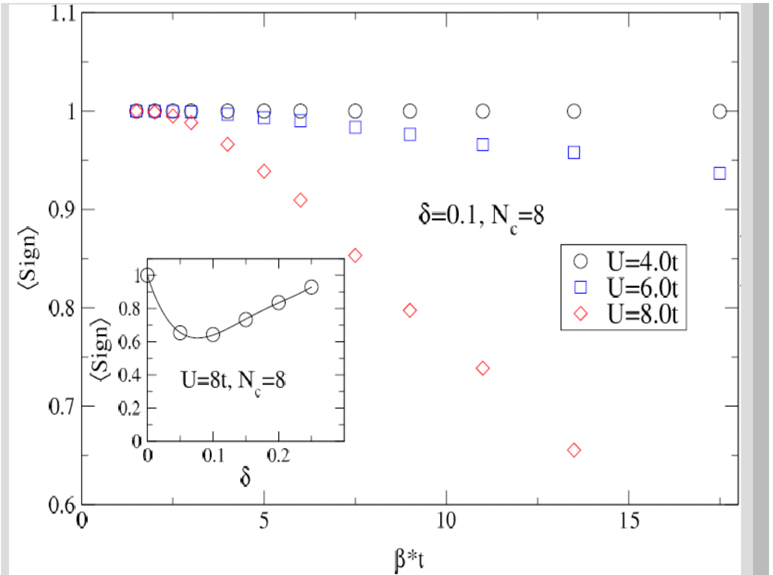
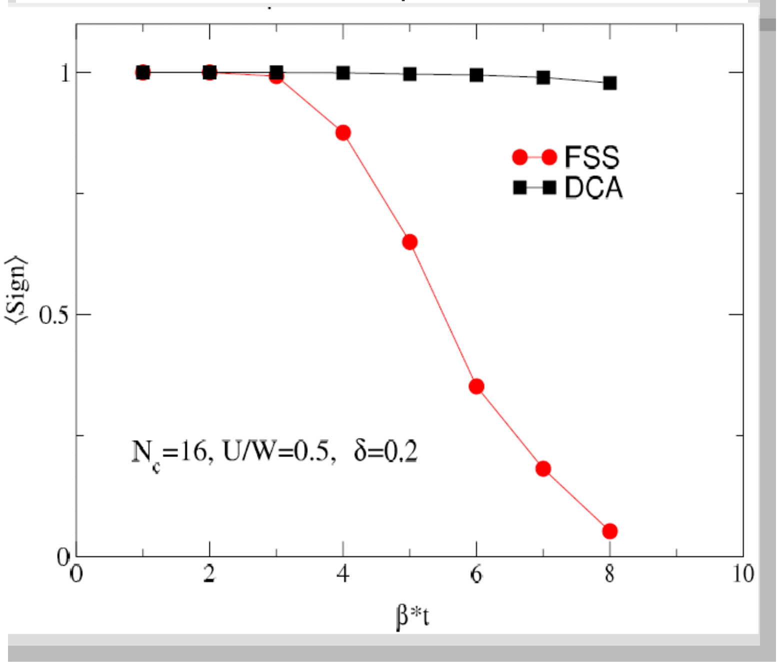
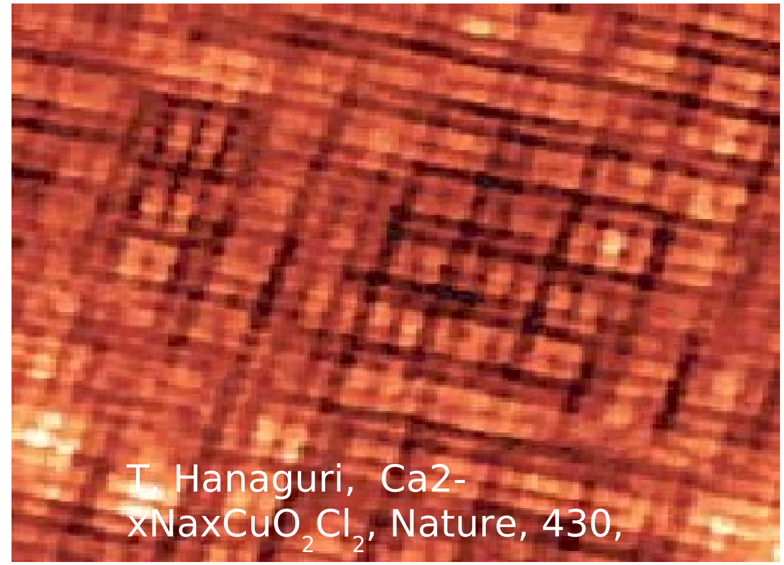
Challenge: QMC sign problem

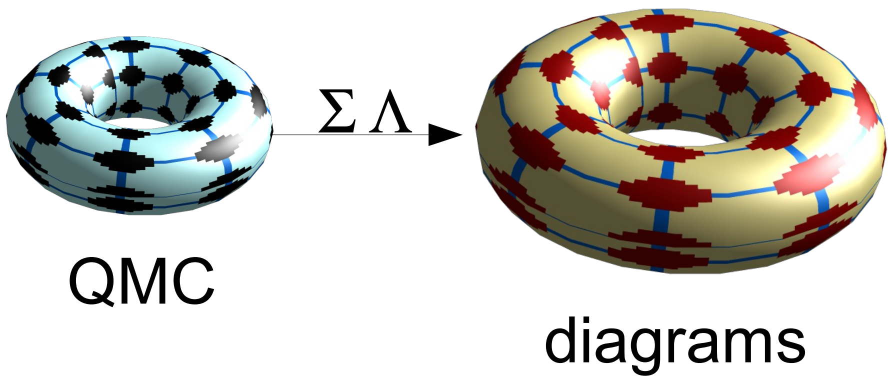






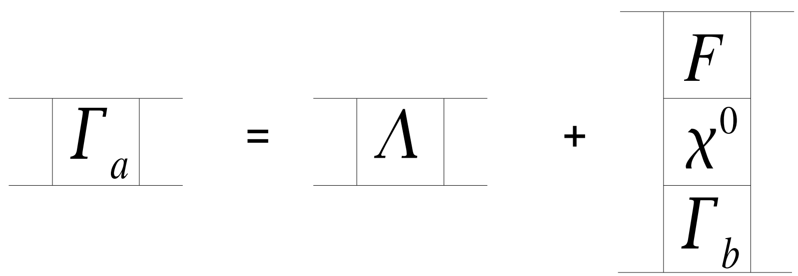
- Repeat length of spin and charge ordering many lattice spacings.
- Sign problem $\langle m\rangle = \langle mS\rangle / \langle S\rangle$.
- Prevents us from treating these long scale correlations explicitly.
- Sign problem is NP hard (M. Troyer, PRL 94, (2005)), $\langle S\rangle$ is big only by accident.
- More computing helps, but ... better algorithms are needed for long lengths!

Diagrammatic Methods at Intermediate Lengths



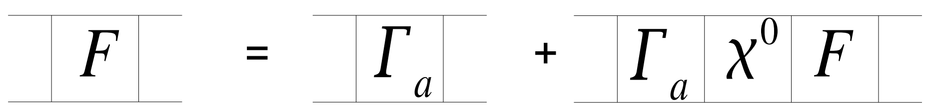
- Causal
- Large cluster: solve parquet and BS equations self consistently.
- Σ, Λ from QMC
- Γ, F, χ size nt >1600 (100G)
- distribute data on Q
- 16,000 proc on Jaguar Xt5 ORNL

Parquet e.q. $\Gamma_a(K,K',Q)=\Lambda(K,K',Q)+(\Gamma_b\chi^0 F)(-K',-K,K+K'+Q)$



Bethe-Salpeter e.q. $F(K,K',Q)=\Gamma_a(K,K',Q)+(F\chi^0\Gamma_a)(K,K',Q)$

N. Bickers
D. Hess
V. Janis
many others



Current and 5-Year Projections

- Current QMC
  - Linear scaling in β, N^3L (improve by a factor of 10^4)
    - Minus sign make true scaling *exp*($N\ \beta$) (**NP hard**)
  - GPU acceleration (improve by 10)
  - Limited to ~20-40 correlated orbitals (certain terms)
- Current diagrammatic parquet
  - Hybrid parallel codes which scale well to > 10^4 cores
    - No minus sign problem
    - True scaling $(NL)^4$
  - Presently limited to ~30 correlated orbitals
    - Number of cores accessible
    - Stability of iterative solution
    - Rank-3 tensor contraction and rotations (MPI all-to-all)
- **Future belongs to multi-scale methods**
  - Limited only by code stability and communication
  - Many possible directions (not just parquet).