Thermodynamics of *d*-wave superconductors: A numerical study based on FLEX and DCA

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Major objectives

- Obtain systematic weak-coupling results (*i.e.* spin fluctuation physics) for the specific heat, C, upper critical field, H_{c2}, etc. by applying the fluctuation exchange approximation (FLEX) to the Hubbard model.
- Determine the extent to which FLEX represents doping-dependence of such properties in the cuprates.
- Assess the general validity of weak-coupling approaches for these systems

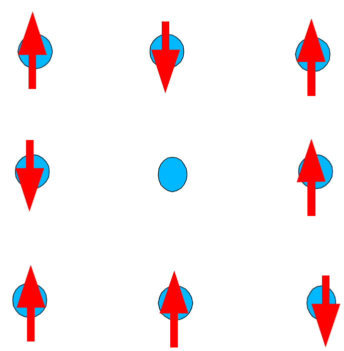
Technical objectives

- Develop a scheme for evaluating diagrams that are typically omitted in FLEX treatments of model *d*-wave superconductors.

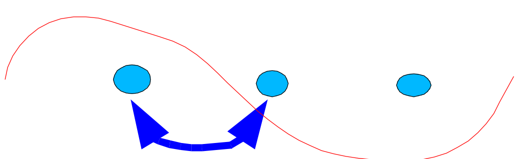
- Evaluate the effectiveness of the dynamic cluster approximation (DCA) as a finite-size scaling technique for numerical studies of *d*-wave superconductivity.

Model Hamiltonian (Hubbard)

- Two-dimensional lattice of atoms, one orbital per unit cell.



n=0.89 (electron filling)



t = hopping = 0.25 eV

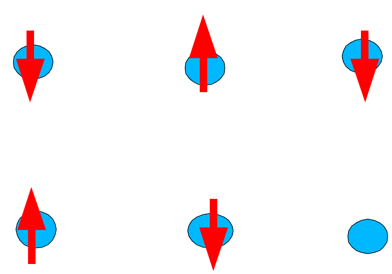
$$E(k) = -2t\,(\,\cos(k_x) + \cos(k_y)\,)$$

Model: interactions

- Energy penalty, *U*, for two electrons at same site

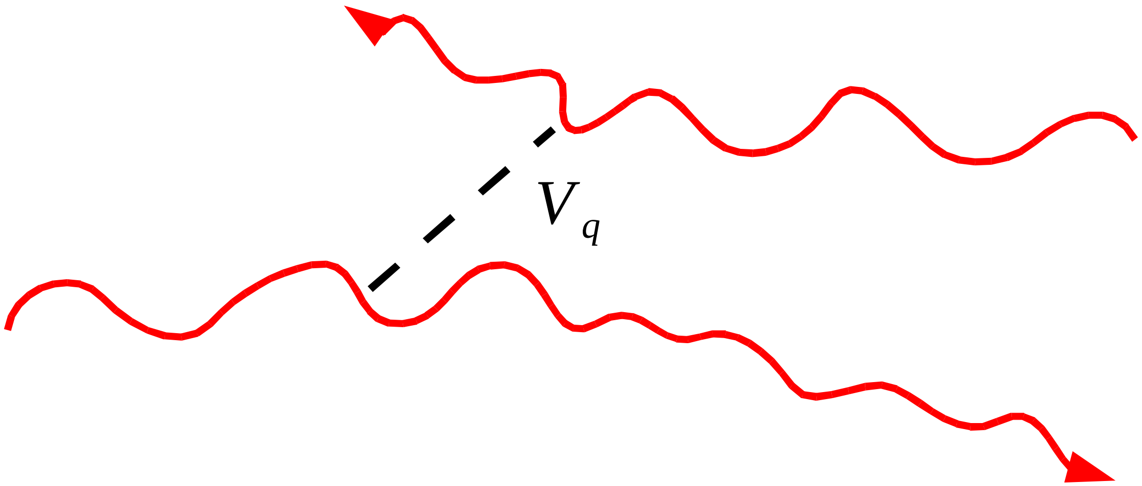
$\Delta E = U$ (1 to 2 eV)

- This favors antiferromagnetic order at n=1 and antiferromagnetic correlations for n values close to 1.

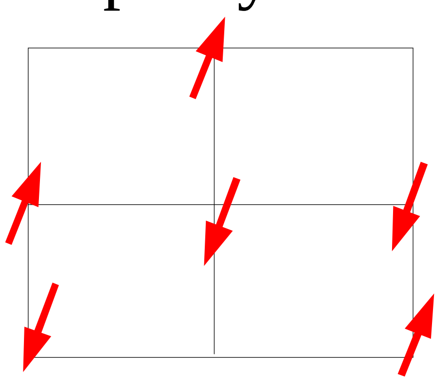


Basic approaches to this model

Weak coupling: interactions are treated perturbatively



Strong coupling: Most important tendency is to avoid double occupancy

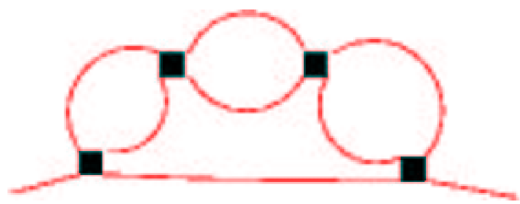


Fluctuation Exchange Approximation (FLEX) for this model

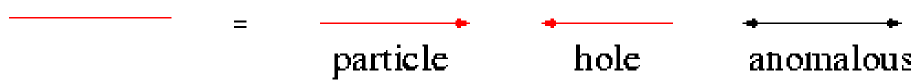
- Weak-coupling based approach (Bickers, White, and Scalapino (1987)).
- Produces a *d*-wave superconducting transition for this model (Pao and Bickers (1994), Monthoux and Scalapino (1994)).
- Weak-coupling, but generates a non-Fermi liquid state above T_c (Deisz, Hess, and Serene (1996)) for electron densities near n=1.

Our implementation of FLEX

- Include *all* fluctuation diagrams generated by the bare scattering vertex (not just the particle-hole type terms).



- Green's functions include all types.

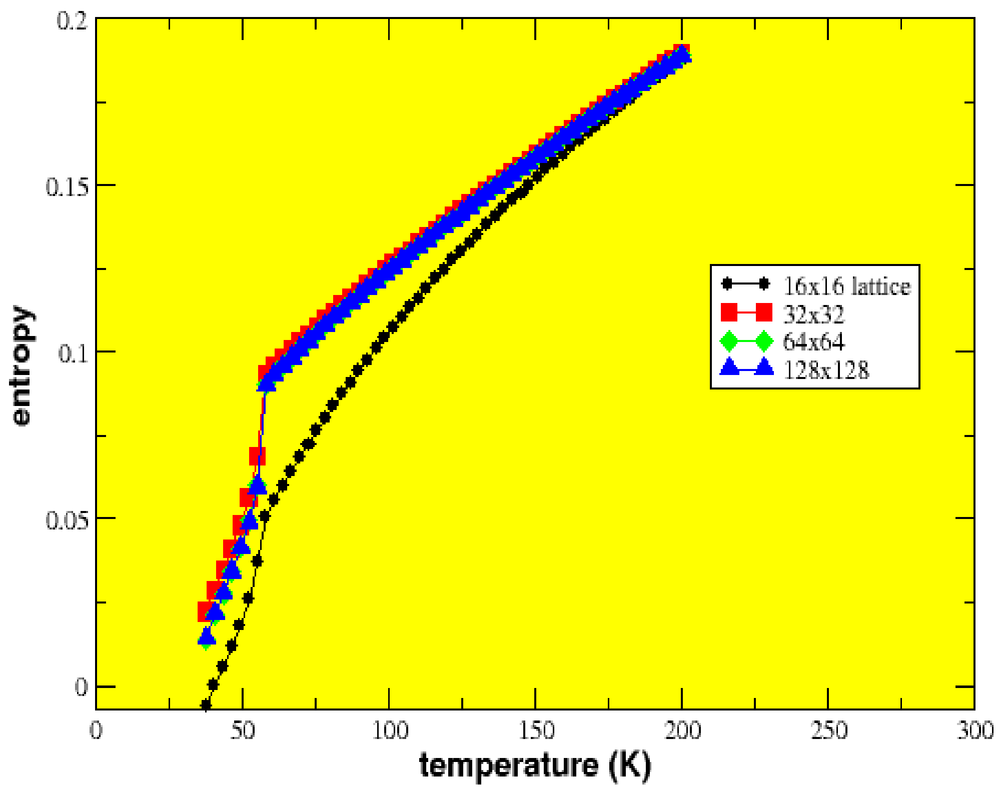


Dynamic Cluster Approximation (DCA) for finite size scaling

- Eliminates level structure effects so as to focus on correlation-induced features in thermodynamics.
  - T_c is relatively small compared to the full bandwidth.
  - Level effects can swamp other features at low T.
- Correlation effects are approximated using finite size clusters (4x4, 8x8, 16x16, etc.)
- Finite-size scaling focuses on size dependence of correlation effects.
- Reference: Hettler, *et al*. (1998)

Example: Treat correlations with a 2x2 cluster.   Combine these correlation effects with level structures obtained from progressively larger lattices.

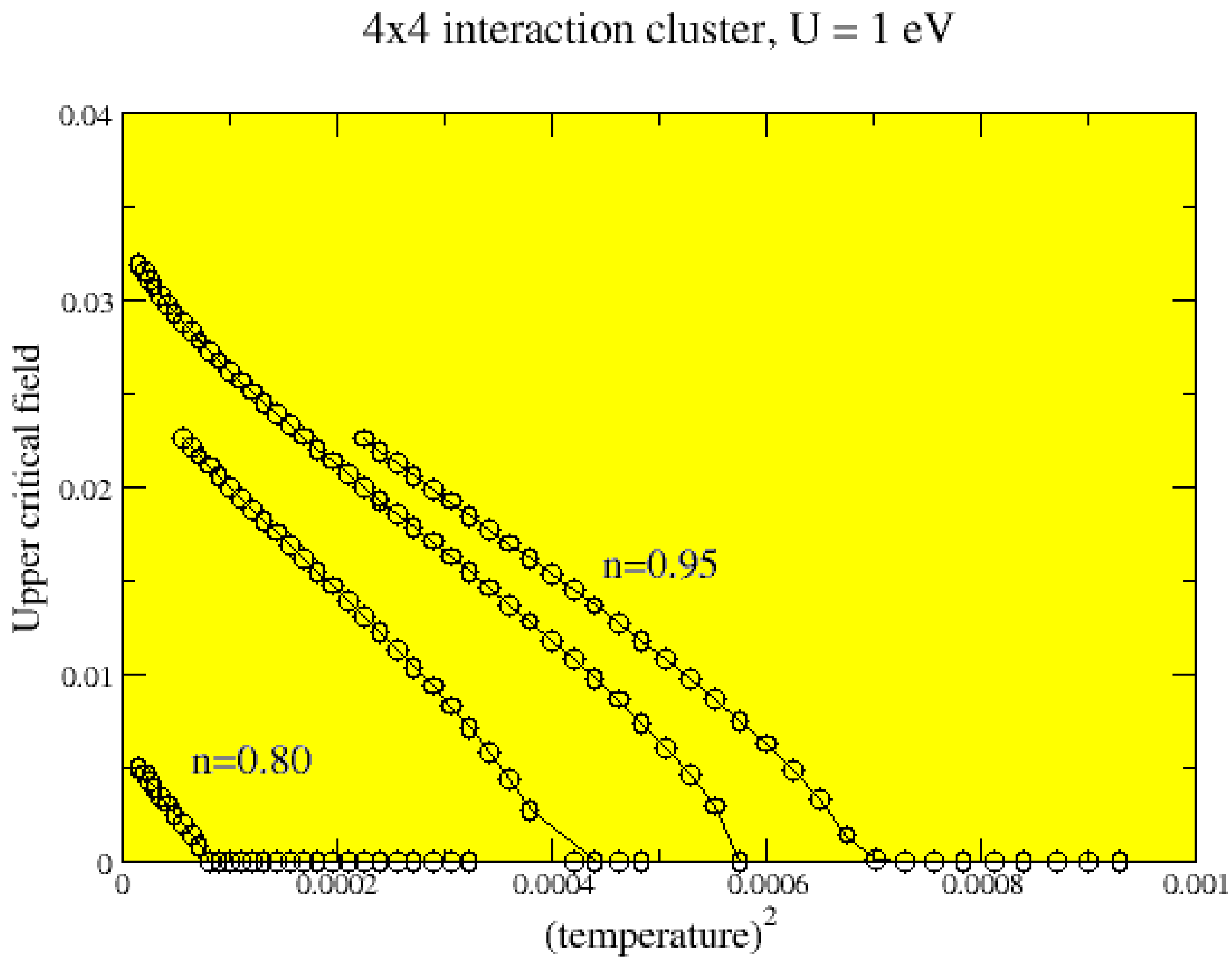
2x2 interaction cluster, n=0.85, U = 1.0 eV



- Large difference between 16x16 and 32x32 lattices due to level structure effects.
- Level structure effects strongly minimized at 64x64.
- Next step, interaction cluster scaling: 2x2 --> 4x4 --> 8x8, etc.

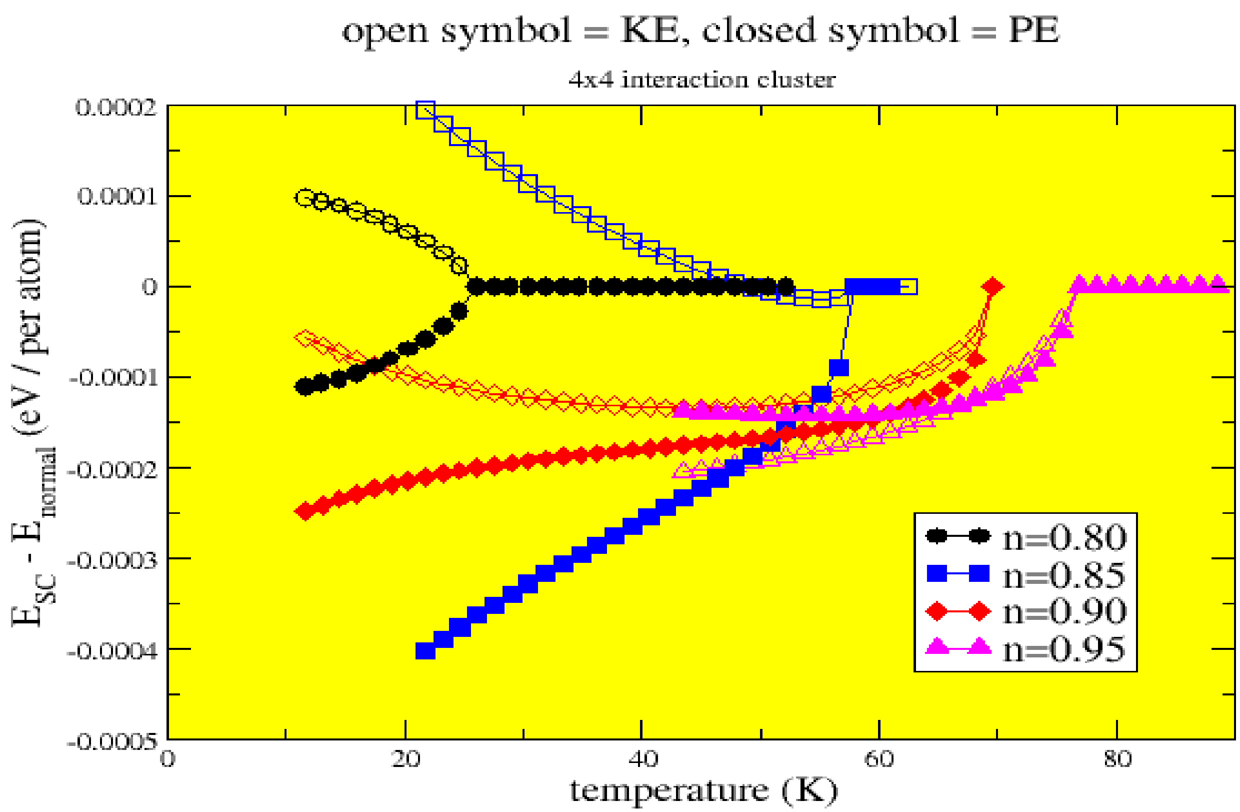
Results

Upper critical field, H_{c2}, versus filling



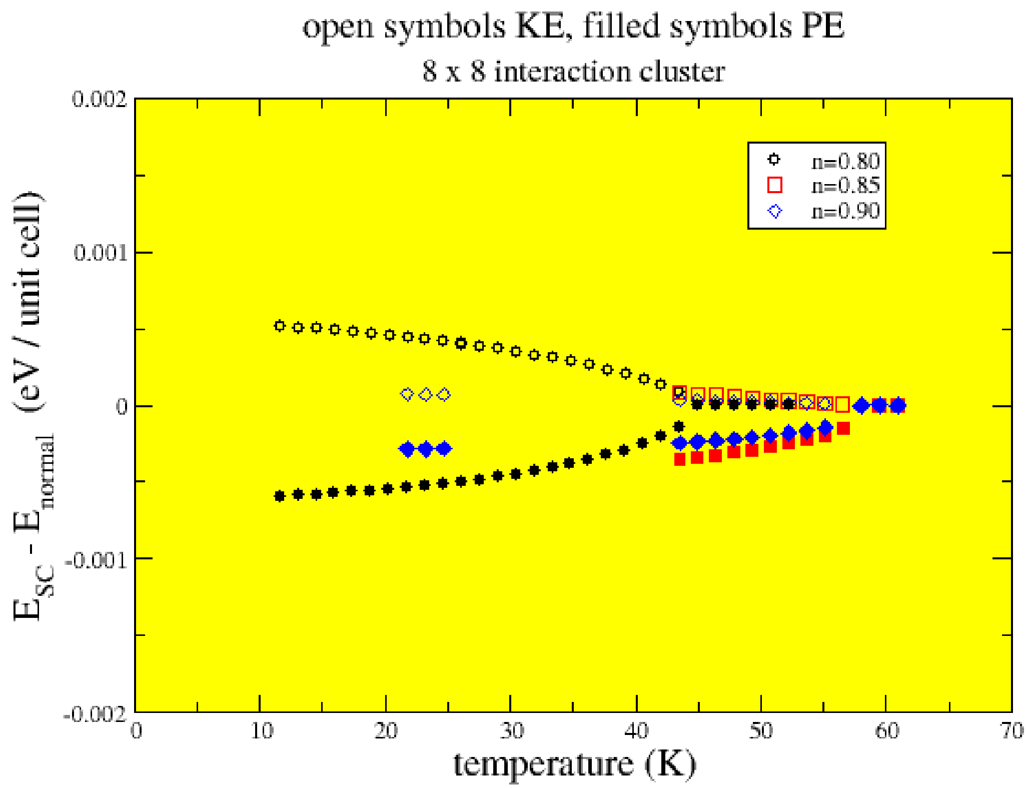
- Standard weak coupling: $H_{c2}(T) \sim 1 - (T / T_c)^2$
- Significant deviations near T_c especially near n=1.

Energetics below Tc: 4x4 interaction cluster



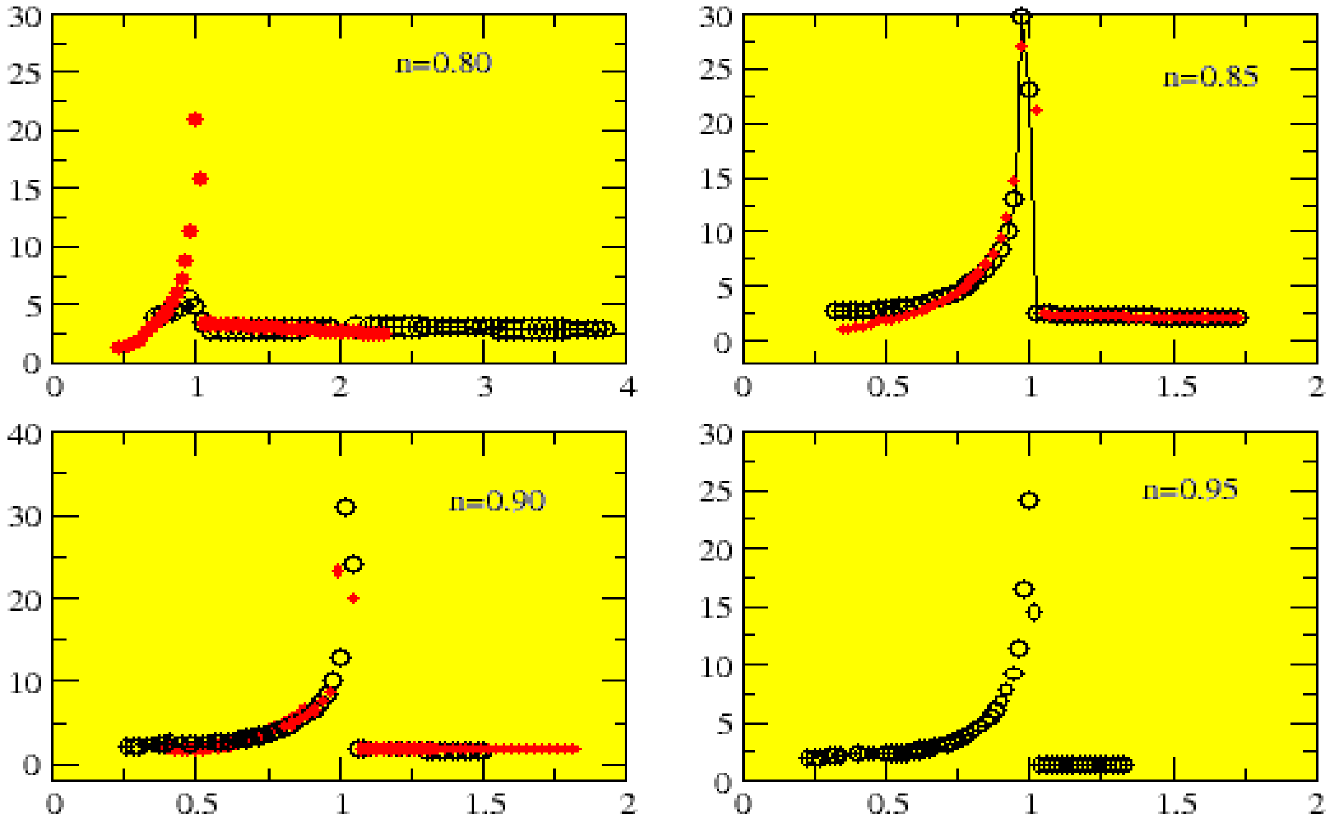
- As density approaches one, KE loss appears to drives the transition, but (next slide) this conclusion changes when a larger interaction cluster is used.
- Transition at lower density (n=0.80) is due to PE loss. This corresponds to the usual scenario for superconductivity.

Energetics below Tc: 8x8 interaction cluster



- According to these weak-coupling results, superconductivity is driven by a potential energy decrease for n < 0.875 for all cluster sizes.
- Results are ambiguous for n > 0.875. Larger clusters are needed to see if kinetic energy decreases with respect to the normal state in the underdoped limit as is observed experimentally.

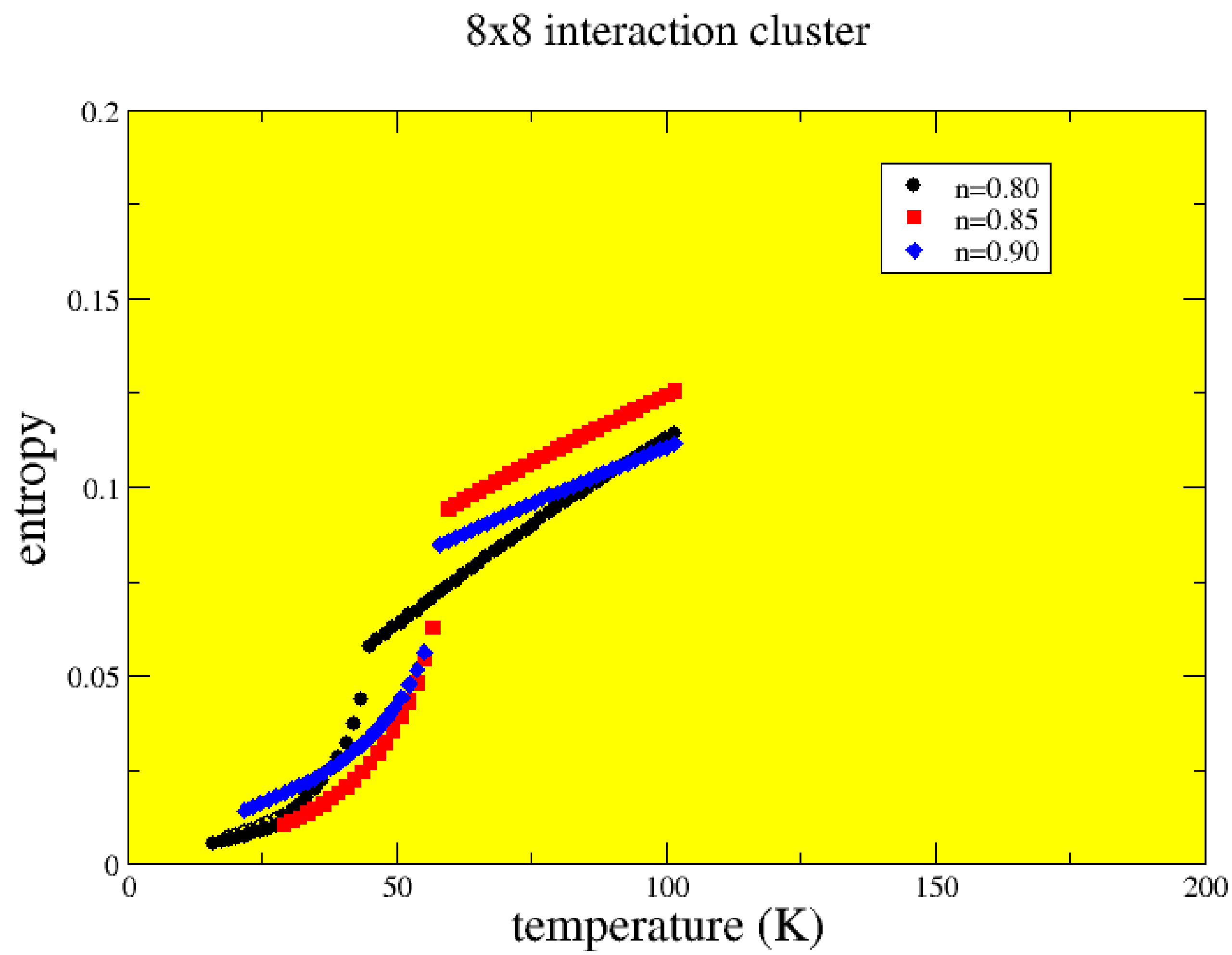
C(T) / T   vs. T / Tc



black = 4x4 cluster, red = 8x8 cluster

- Non-BCS-like behavior near Tc. Perhaps due to the rapid opening of the superconducting gap below Tc (Pao and Bickers (1994).

- Suppressed normal state specific heat for n=0.95 on account of the normal state pseudogap.



- Likewise the normal state entropy is somewhat suppressed near n=1.00.

Future directions

- Layered systems and other lattice structures
- Fluctuation effects in *s*-wave superconductors
- Microscopically based treatment of correlations and disorder in *d*-wave superconductors.