How d-wave Pair Fluctuations Develop from Strong Electronic Correlations

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Models and singlet pairs

$$H = -tP \sum_{\langle ij \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) P + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$H = -t \sum_{\langle ij \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Only spin singlet pairs are considered:

$$\Delta_{ij} = \frac{1}{\sqrt{2}} \left(c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} \right)$$

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Method of Calculation: High Temperature Series Expansion

Series Expansions are linked cluster expansions. For each cluster we calculate the Hermitian pair correlator to 12th order in β

$$\frac{1}{2}\langle \Delta^\dagger_{ij}\Delta_{kl} + \Delta^\dagger_{lk}\Delta_{ji}\rangle$$

Problem: This four-point correlator contains products of lower order correlators as well as the pair fluctuations we want.

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Pair Cumulant

Remove the disconnected pieces

$$\begin{aligned}
\mathcal{P}(i,j,k,l) &= \frac{1}{2}\langle \Delta^\dagger_{ij}\Delta_{kl} + \Delta^\dagger_{lk}\Delta_{ji}\rangle \\
&- \frac{1}{4}\Big[\langle c^\dagger_{i\downarrow}c_{l\downarrow}\rangle\langle c^\dagger_{j\uparrow}c_{k\uparrow}\rangle + \langle c^\dagger_{i\downarrow}c_{k\downarrow}\rangle\langle c^\dagger_{j\uparrow}c_{l\uparrow}\rangle \\
&+\langle c^\dagger_{i\uparrow}c_{l\uparrow}\rangle\langle c^\dagger_{j\downarrow}c_{k\downarrow}\rangle + \langle c^\dagger_{i\uparrow}c_{k\uparrow}\rangle\langle c^\dagger_{j\downarrow}c_{l\downarrow}\rangle \\
&+\langle c^\dagger_{l\downarrow}c_{i\downarrow}\rangle\langle c^\dagger_{k\uparrow}c_{j\uparrow}\rangle + \langle c^\dagger_{k\uparrow}c_{i\uparrow}\rangle\langle c^\dagger_{l\downarrow}c_{j\downarrow}\rangle \\
&+ \langle c^\dagger_{l\uparrow}c_{i\uparrow}\rangle\langle c^\dagger_{k\downarrow}c_{j\downarrow}\rangle + \langle c^\dagger_{k\downarrow}c_{i\downarrow}\rangle\langle c^\dagger_{l\uparrow}c_{j\uparrow}\rangle\Big]
\end{aligned}$$

For a non-interacting model $\mathcal{P}(i,j,k,l) = 0$

Correlation Length

By embedding the clusters in the square lattice we produce the pair correlator per site $\mathcal{P}(\mathbf{r}, \mathbf{r}', \mathbf{R})$, where $\mathbf{R}$ is a measure of the distance between the two pairs. From this and symmetry factors we construct an effective two-point correlator $P_\alpha(\mathbf{R})$ which can be used to calculate the Q=0 pair correlation length

$$\xi_\alpha^2 = \frac{1}{2d}\frac{\sum_{\mathbf{R}} |\mathbf{R}|^2 P_\alpha(\mathbf{R})}{\sum_{\mathbf{R}} P_\alpha(\mathbf{R})}$$

How should the effective two-point correlator be calculated?

•The effective two-point correlator must be consistent with Ginzburg-Landau theory of order parameter fluctuations

•Change in the zero field free energy:

$$\Delta F = \int d^3\mathbf{R}\left[\alpha|\eta|^2 + \beta|\eta|^4 + K_1|\vec{\nabla}\eta|^2\right]$$

where the order parameter is a function of position and Temperature, $\eta(\mathbf{R},T)$

•The order parameter is related to the two-point correlator

$$P(\mathbf{Q}) = \left\langle\left|\eta(\mathbf{Q},T)\right|^2\right\rangle$$

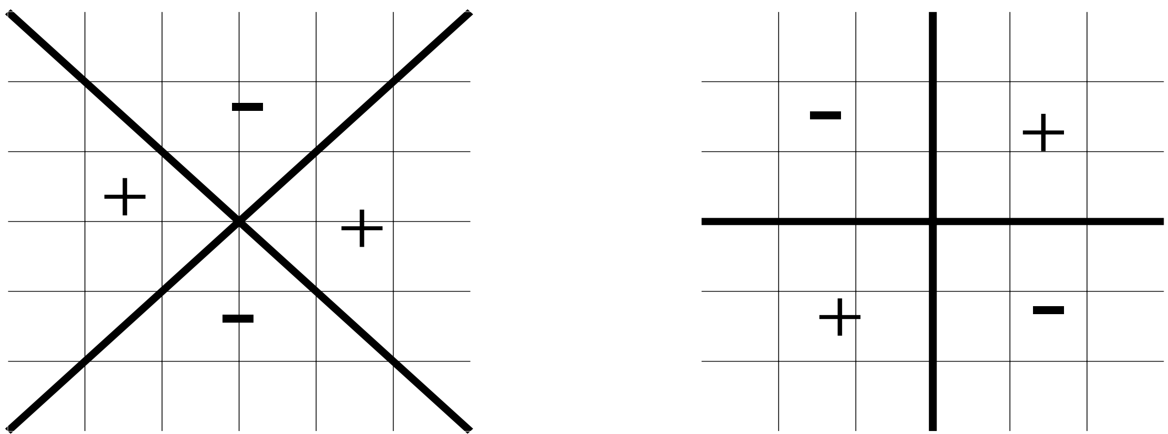
•The momentum dependent two-point correlator must be non-negative and cannot depend on the internal pair phase

Pair Symmetry Functions

We now need to include symmetry factors

$\phi_\alpha($ … d_{xy}

and … 1.



Effective Two-Point Correlator

- The full four-point correlator defines a matrix for a fixed $\mathbf{R}$:

$$M_{\alpha\mathbf{R}}(\mathbf{r},\mathbf{r}') = \phi_\alpha(\mathbf{r})\phi_\alpha(\mathbf{r}')\mathcal{P}(\mathbf{r},\mathbf{r}',\mathbf{R})$$

- The effective two-point correlator is found as the trace of this matrix:

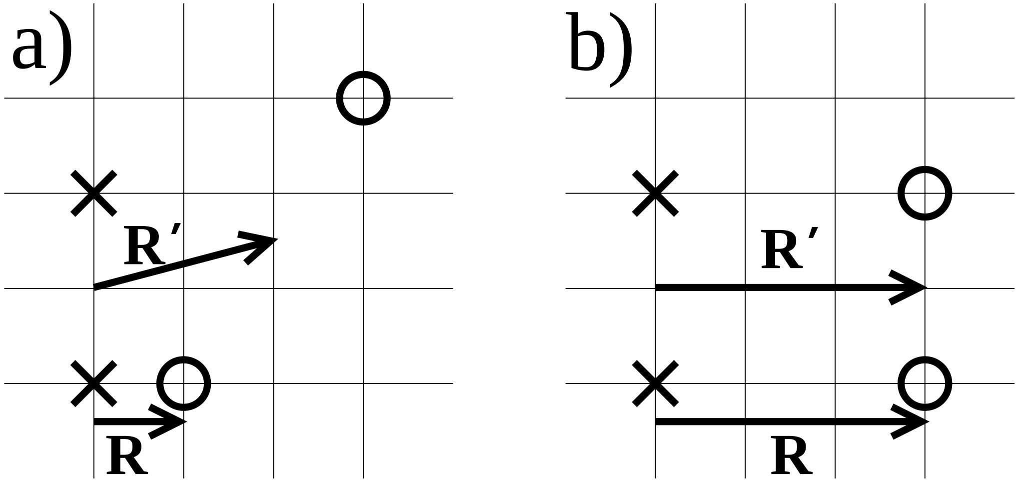
$$P_\alpha(\mathbf{R}) = \mathrm{Tr}_{\mathbf{r}} M_{\alpha\mathbf{R}}(\mathbf{r},\mathbf{r}')$$

Pairs a

- In general there is no unique way to specify the distance between pairs

R’: CM to CM

R: end to end



- The trace is invariant under different definitions of R

Properties of the Effective Two-Point Correlator

- In terms of the details of the four-point correlator, the effective two-point correlator is

$$P_\alpha(\mathbf{R}) = \sum_{\mathbf{r}} \phi_\alpha^2(\mathbf{r}) \mathcal{P}(\mathbf{r}, \mathbf{r}, \mathbf{R})$$

- Thus to distinguish different pair symmetries we must be sensitive to the **nodes** of the pair wave function
- The contributions to the pair wave function beyond nearest neighbors are important

Exact Expression for P(R=0)

- The R=0 pair correlator can be written exactly as a sum of two-point correlators

$$P_\alpha(\mathbf{R}=0) = \sum_{\mathbf{r}}{}' \left[-\frac{3}{4} \langle S_0^z S_{\mathbf{r}}^z \rangle + \frac{1}{2} \left[\langle n_0 n_{\mathbf{r}} \rangle - n^2 \right] - \left| \left\langle c_0^\dagger c_{\mathbf{r}} \right\rangle \right|^2 \right]$$

where the prime removes r's on nodes for symmetry α

- For $d_{x^2-y^2}$ symmetry $-\frac{3}{4}\sum_{\mathbf{r}}{}' \langle S_0^z S_{\mathbf{r}}^z \rangle$ diverges in the ordered antiferromagnet due to the d-wave nodes removing only FM aligned spins

P(R=0) Continued

- One must be very careful in determining the presence of d-wave superconducting fluctuations to not be fooled by a large value of $P_d(R=0)$
- Need to find a peak around Q=0 (or the equivalent) that narrows and grows with reducing the temperature
- Q=0 correlators or momentum sums of correlators can diverge without pair fluctuations being present

Prior Calculations

The correlator used in earlier unbiased calculations typically has the form

$$D_d(\mathbf{R}) = \left\langle \Delta_d^\dagger(0)\Delta_d(\mathbf{R}) \right\rangle$$

where $\Delta_d^\dagger(\mathbf{R}) = \frac{1}{2}\sum_\delta g_d(\delta)\left(c^\dagger_{\mathbf{R}+\delta\uparrow}c^\dagger_{\mathbf{R}\downarrow} - c^\dagger_{\mathbf{R}+\delta\downarrow}c^\dagger_{\mathbf{R}\uparrow}\right)$
with

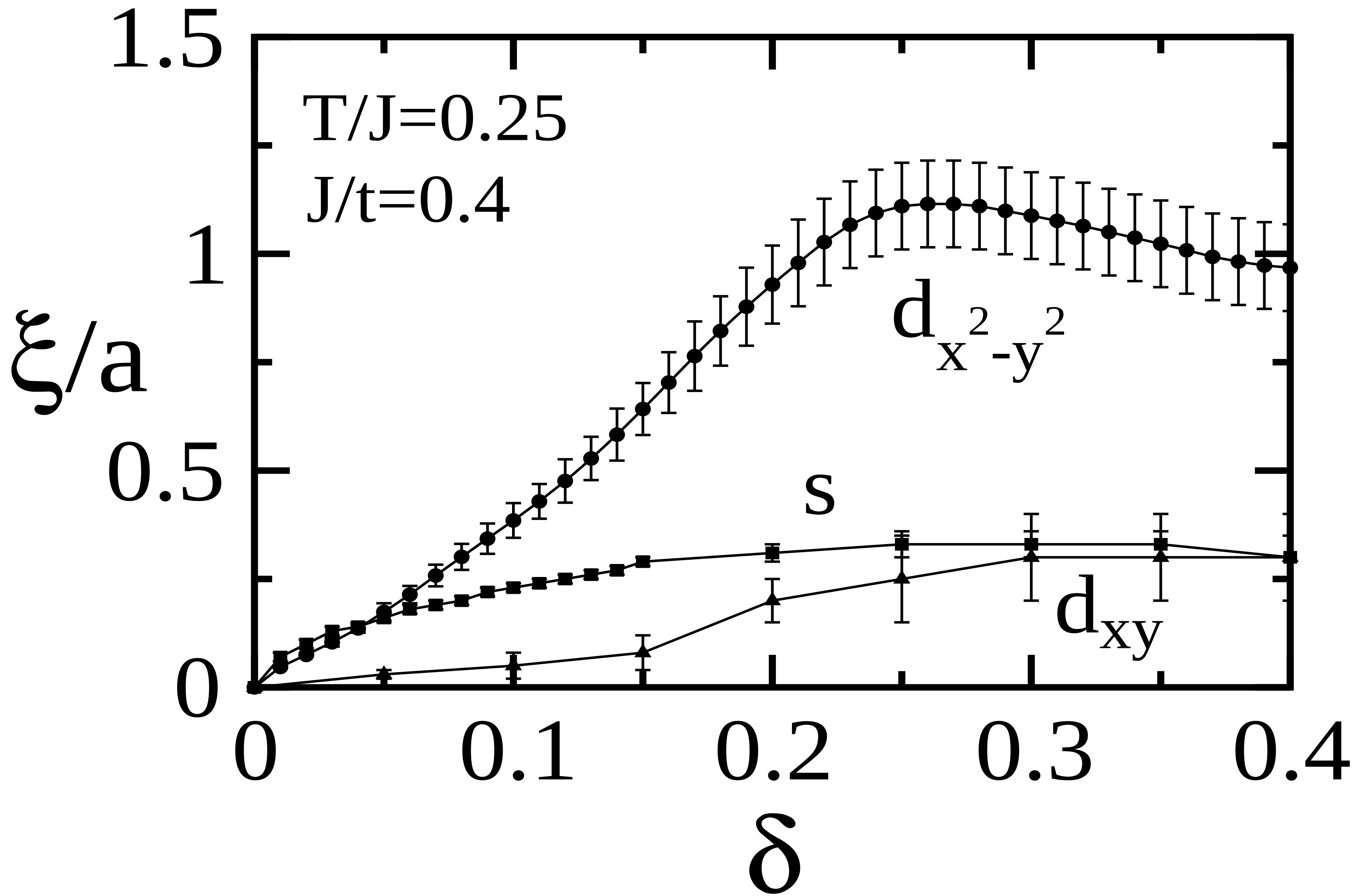
$g_d(\delta) = +1$ for $\delta = \pm\hat{\mathbf{x}}$

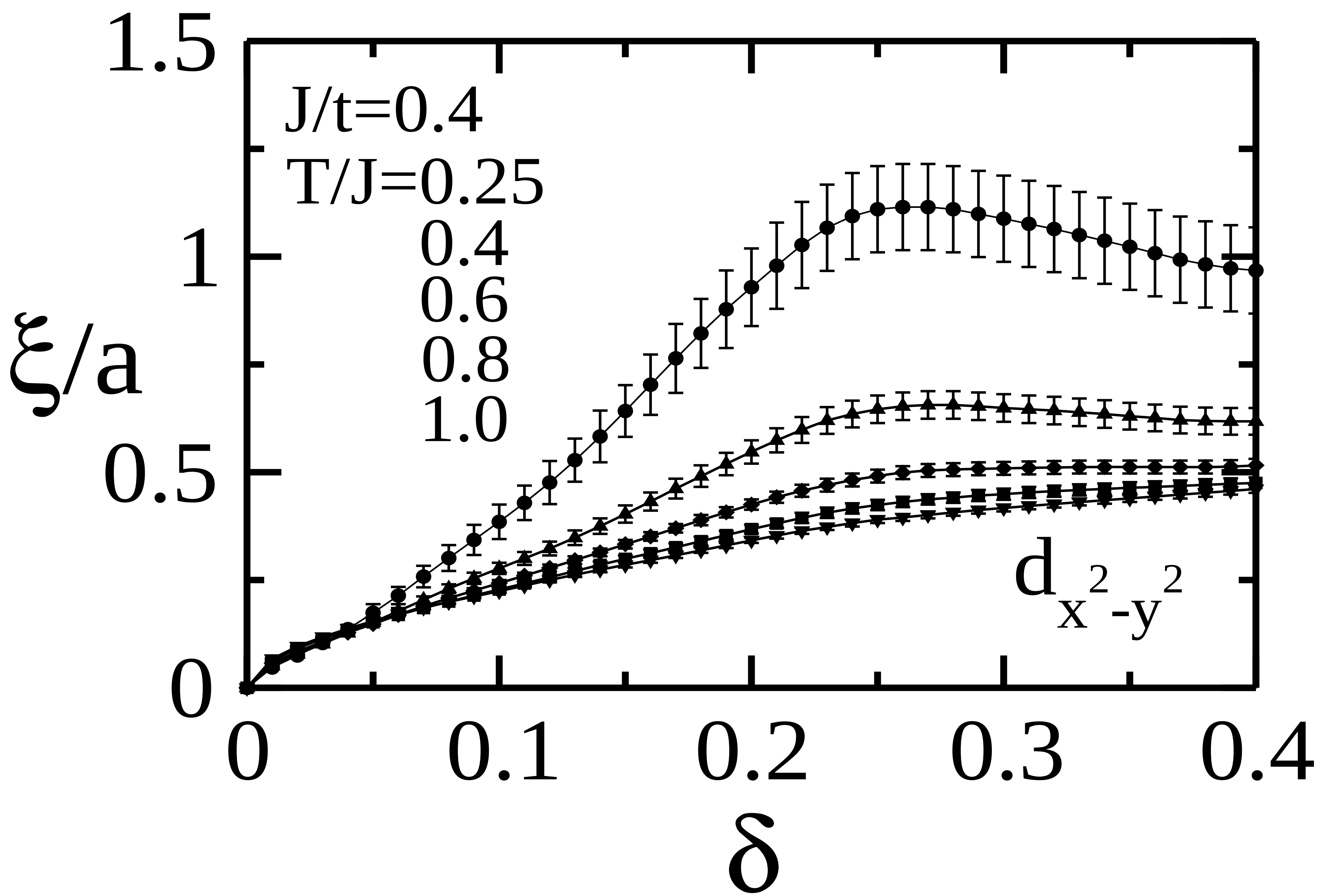
and $g_d(\delta) = -1$ for $\delta = \pm\hat{\mathbf{y}}$

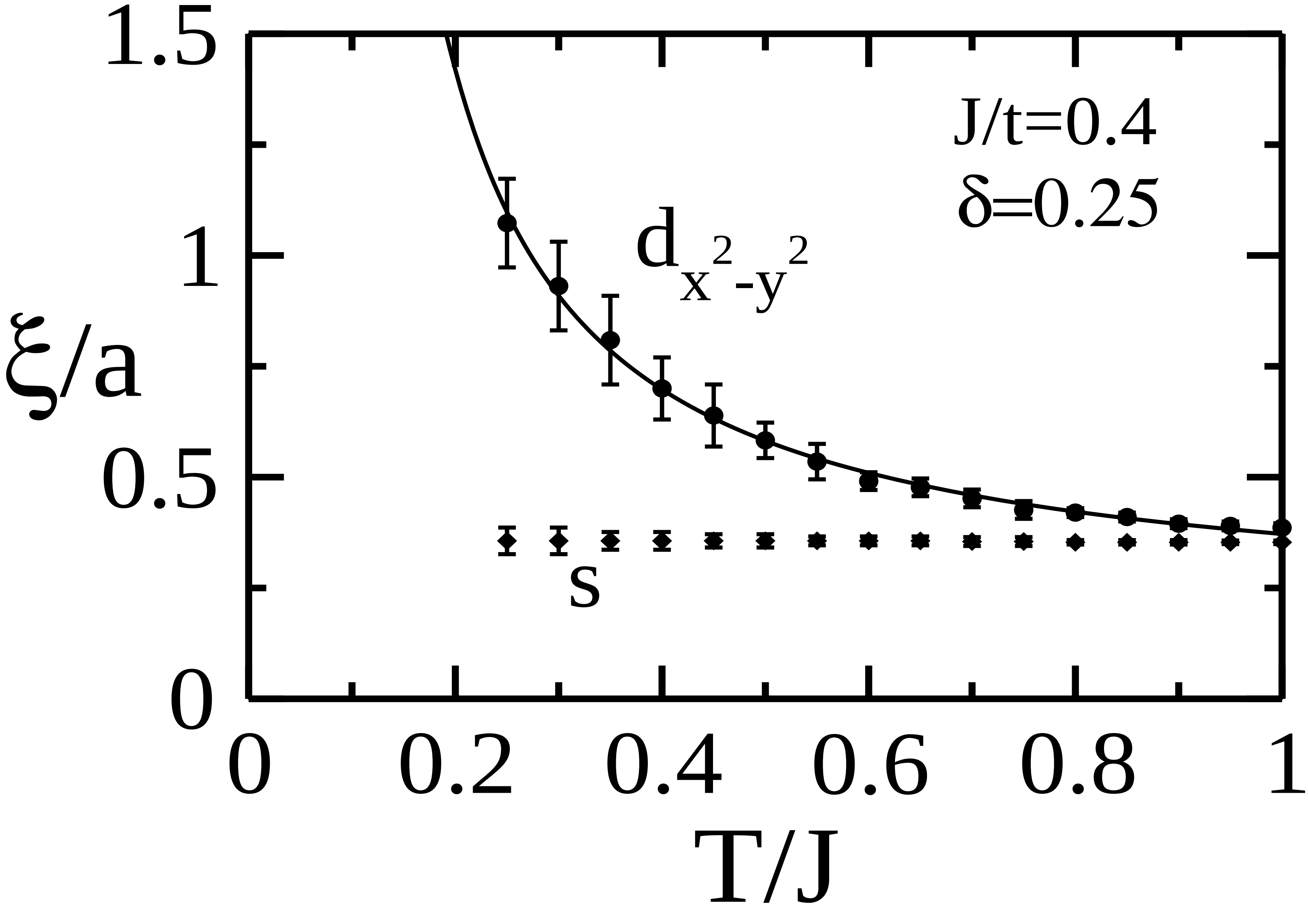
Prior, continued

- Doesn’t remove disconnected pieces of the four-point correlator
- Effective two-point correlation function depends on internal phase – not consistent with GL
- Restricted to nn, not sensitive to nodes
- Inconsistent labeling of position of pairs
- Frequently, only the Q=0 correlator is used or only momentum sums are used

WO Putikka and MU Luchini, PRL96, 247001 (2006)




J/t=0.4
T/J=0.25
0.4
0.6
0.8
1.0
$d_{x^2-y^2}$
ξ/a
δ
1.5
1
0.5
0
0
0.1
0.2
0.3
0.4



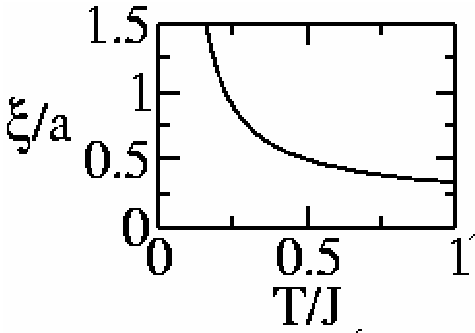
1.5
1
0.5
0
ξ/a
J/t=0.4
δ=0.25
$d_{x^2-y^2}$
s
0
0.2
0.4
0.6
0.8
1
T/J

Effect of Superconducting Fluctuations on Single Particle Properties

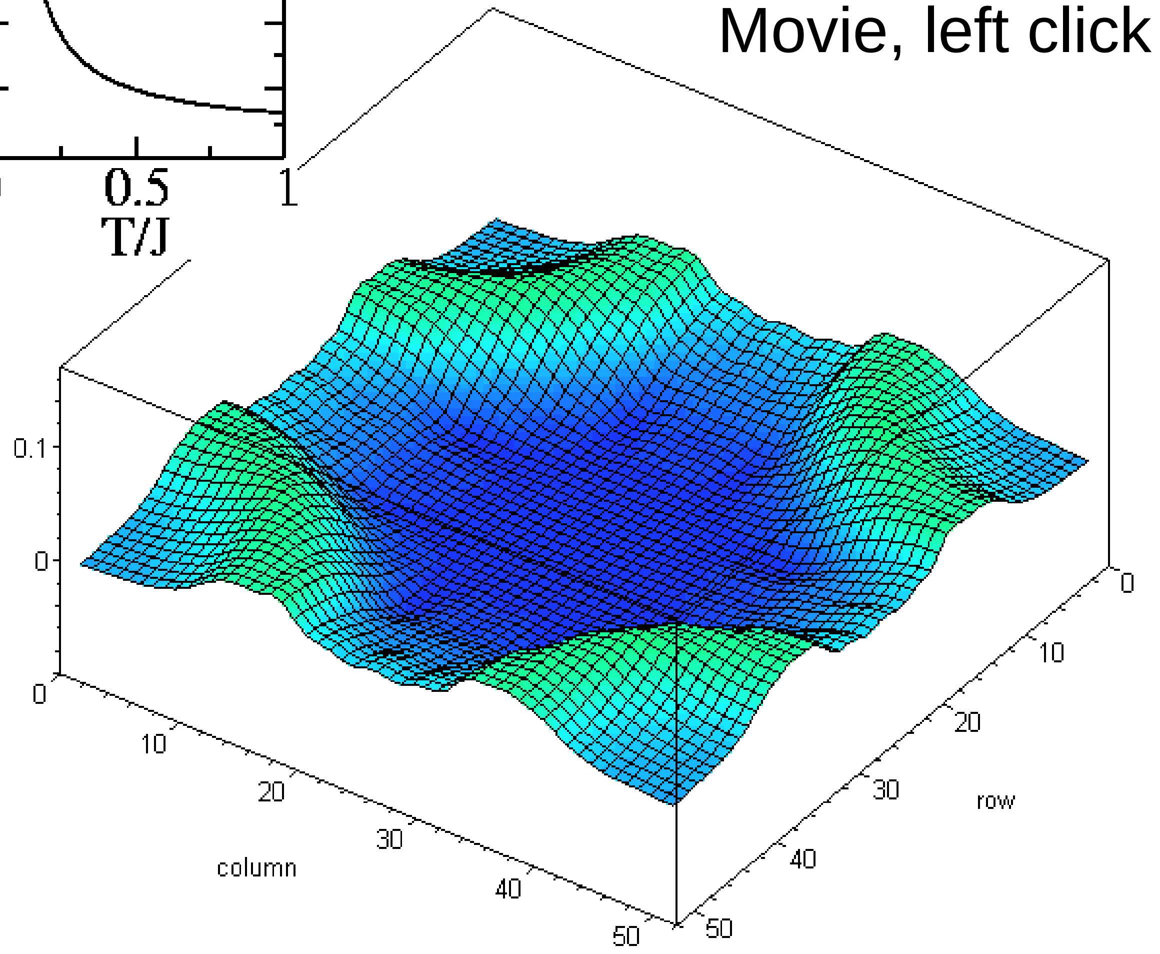
- Superconducting fluctuations should affect the low energy single particle spectrum.
- The temperature derivative of the momentum distribution for a BCS superconductor at low temperatures suggests

$$\frac{dn_{\mathbf{k}}}{dT} \propto \frac{1}{|\Delta_{\mathbf{k}}|}$$

WOP, MU Luchini and RRP Singh, PRL 81, 2966 (1998)



Movie, left click to play



$$\frac{dn_{\mathbf{k}}}{dT}$$

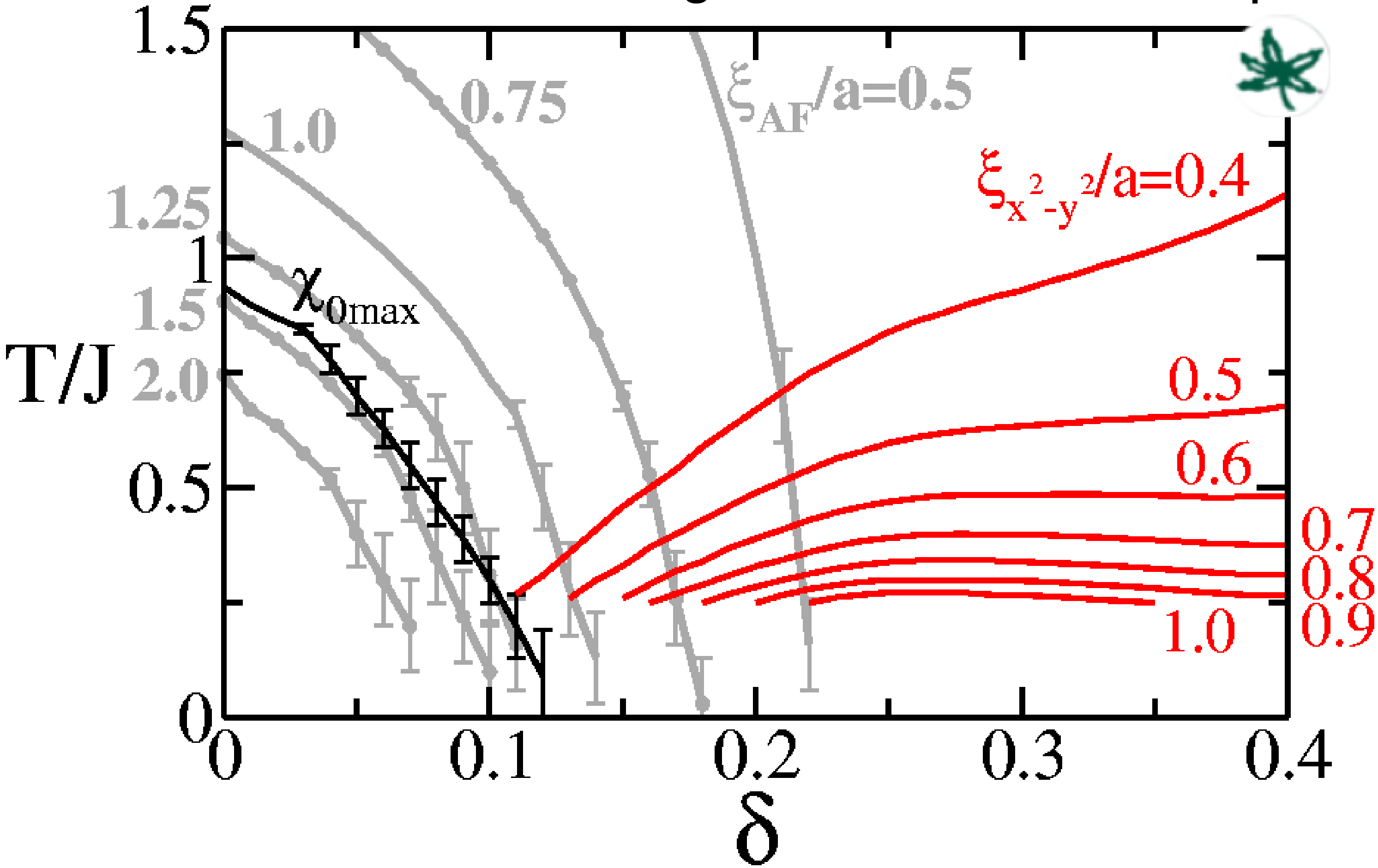
$$J/t = 0.4$$

$$\delta = 0.20$$

Relation to the Pseudogap

Another possiblity for the peaks in $dn_{\mathbf{k}}/dT$ is the pseudogap, which is also expected to have nodes on the BZ diagonal. We can use the maximum in the uniform spin susceptibility as a function of temperature as a marker for the pseudogap. The pseudogap boundary is a plot of $\chi_{0\mathsf{max}}$ on a (δ, T) phase diagram.

T. Koretsune, M. Ogata and WOP, to be published



•No overlap of pseudogap and strongest SC fluctuations

Comparison to real high Tc Superconductors

Real high Tc materials have longer range interactions (t',J', etc.) that have not been included in the current calculation.

How large does $\xi_{x^2-y^2}$ have to be to produce true 3D order? For a rough estimate we can use

$$V_{ij}(\xi_{x^2-y^2}/a)^2 \approx T_{\mathrm{C}}$$

What Properties of Strong Correlations Lead to d-wave Pair Fluctuations?

- Usual approach: Use fluctuations in some other order parameter to create an interaction that produces pair fluctuations
- Problem: Why doesn’t the stronger fluctuation order instead of superconductivity?
- Alternative: The pair fluctuations arise directly from the strong correlations
- <u>All</u> types of order parameter fluctuations compete to order the system

Trivial, but Important, Point

- Whatever the mechanism leading to superconducting fluctuations, it must exist for temperatures at or above the temperature where the SC fluctuations start to grow
- From the pair correlator we *know* this temperature is ~J/2 at n = 0.8.
- Need to consider what is happening at higher temperatures first before trying to identify the possible low temperature fluctuations

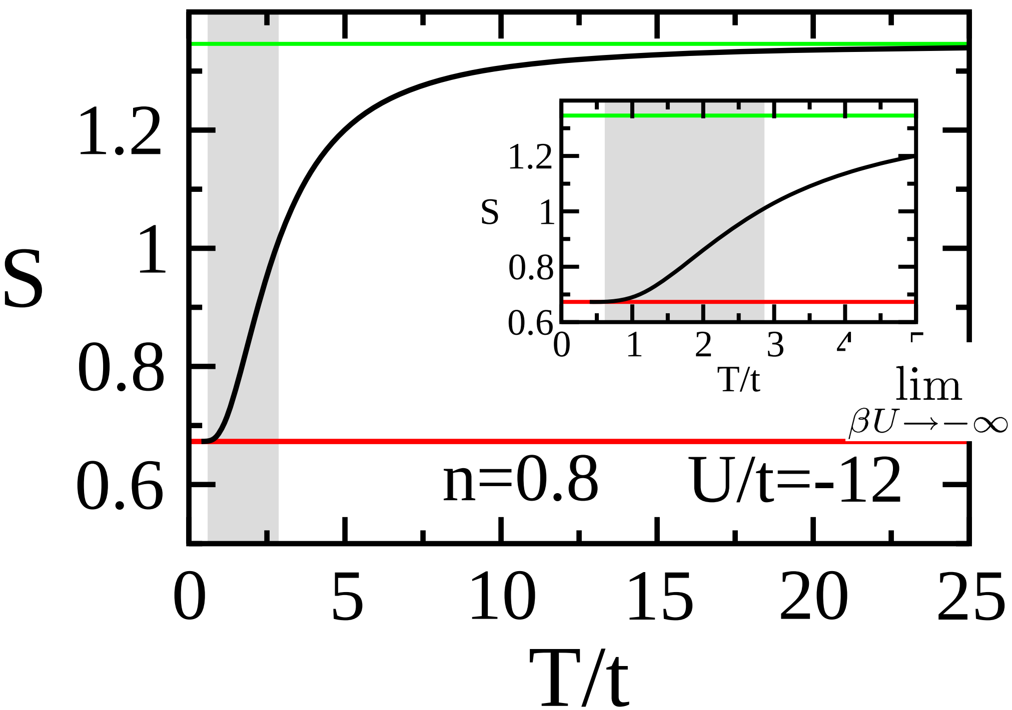
Hubbard Model Degrees of Freedom

- To determine what fluctuations can develop at low temperatures, first identify the degrees of freedom at higher temperatures
- Use the high temperature entropy to identify the degrees of freedom
- Consider the limit $|U/t| \gg 1$, $T/t \gg 1$ where the single site approximation is good

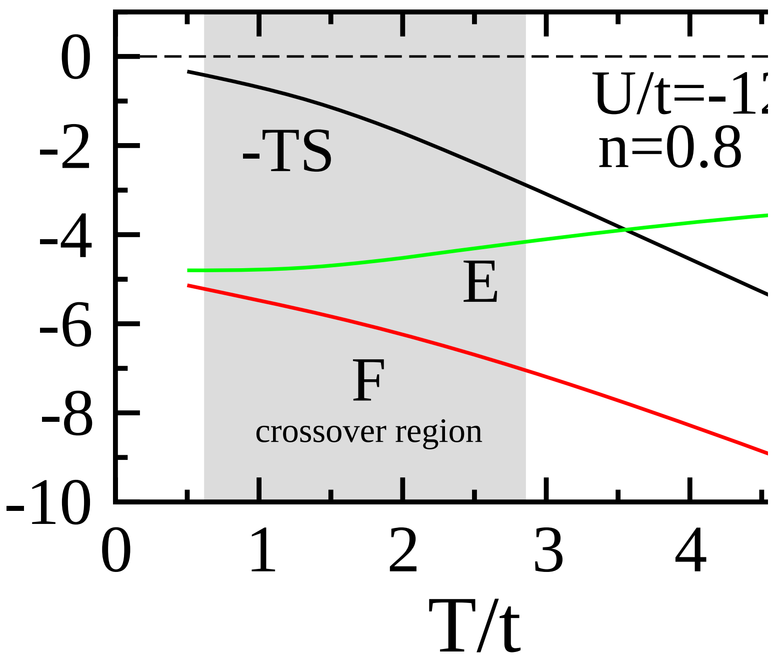
Negative U Hubbard Model

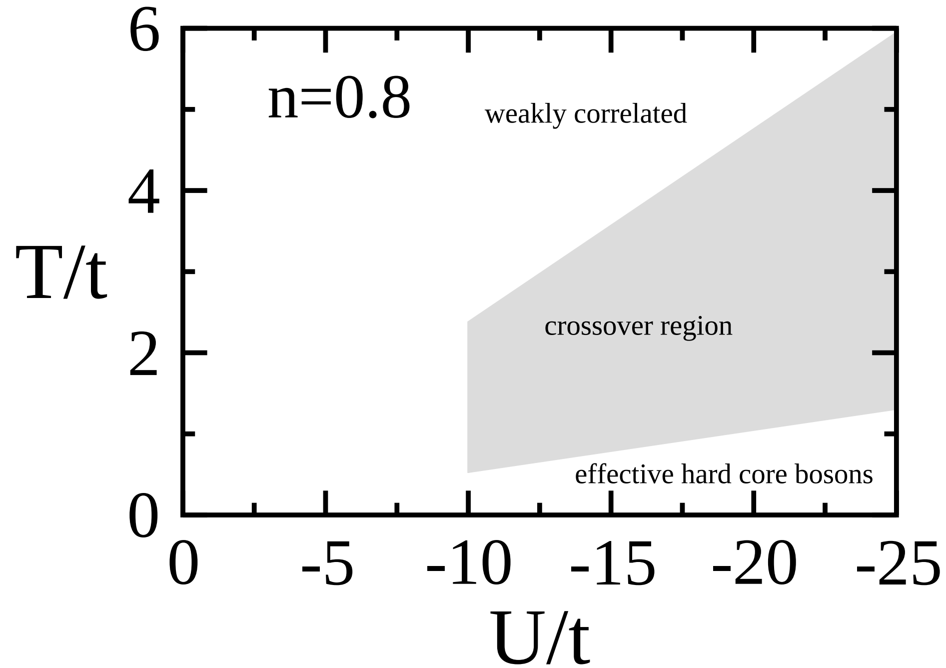
- Well known crossover to hard core bosons

$$\lim_{\beta U \to 0} S = 2\left[-\frac{n}{2}\log\left(\frac{n}{2}\right) - \left(1-\frac{n}{2}\right)\log\left(1-\frac{n}{2}\right)\right]$$



$$\lim_{\beta U \to -\infty} S = -\frac{n}{2}\log\left(\frac{n}{2}\right) - \left(1-\frac{n}{2}\right)\log\left(1-\frac{n}{2}\right)$$



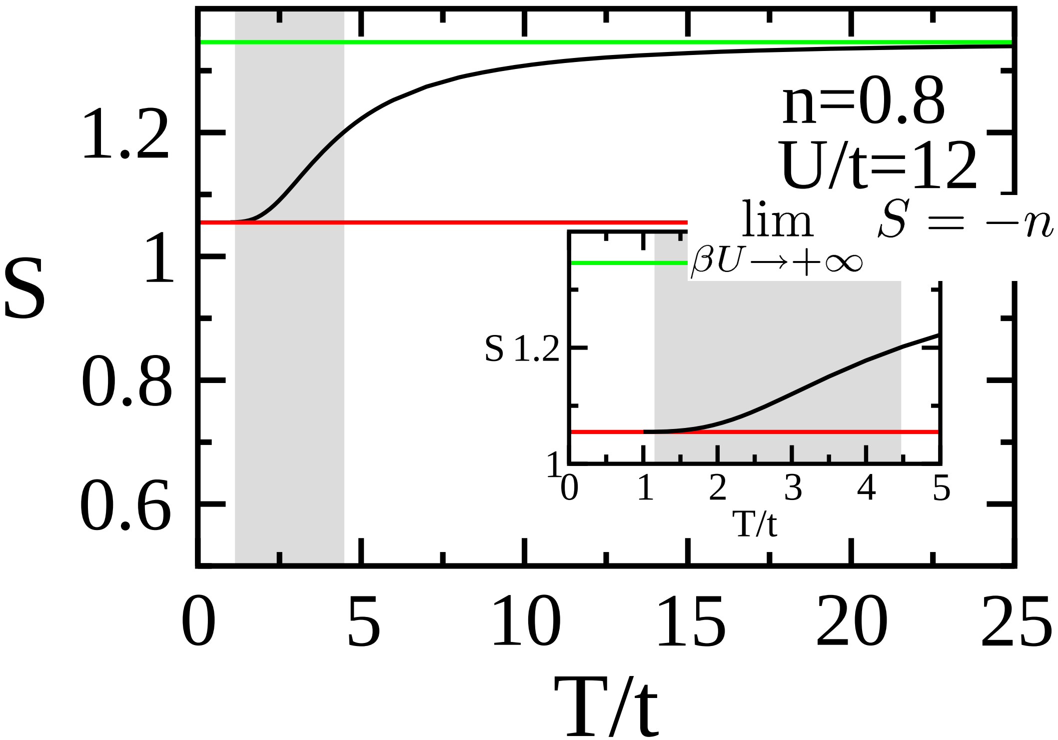


- The free energy F = E – TS is dominated by the internal energy in the crossover temperature range
- Below the crossover there are effective hard core bosons with half the original electron density

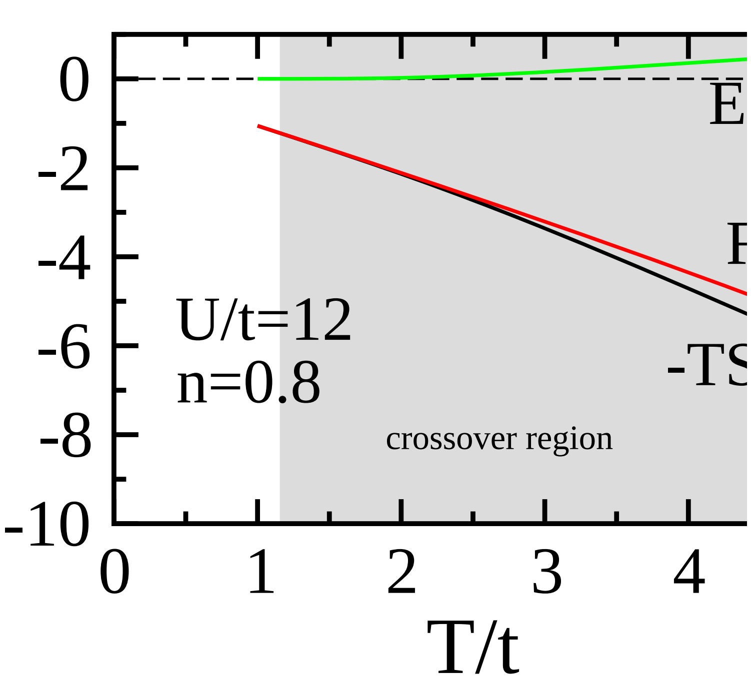
Positive U Hubbard Model

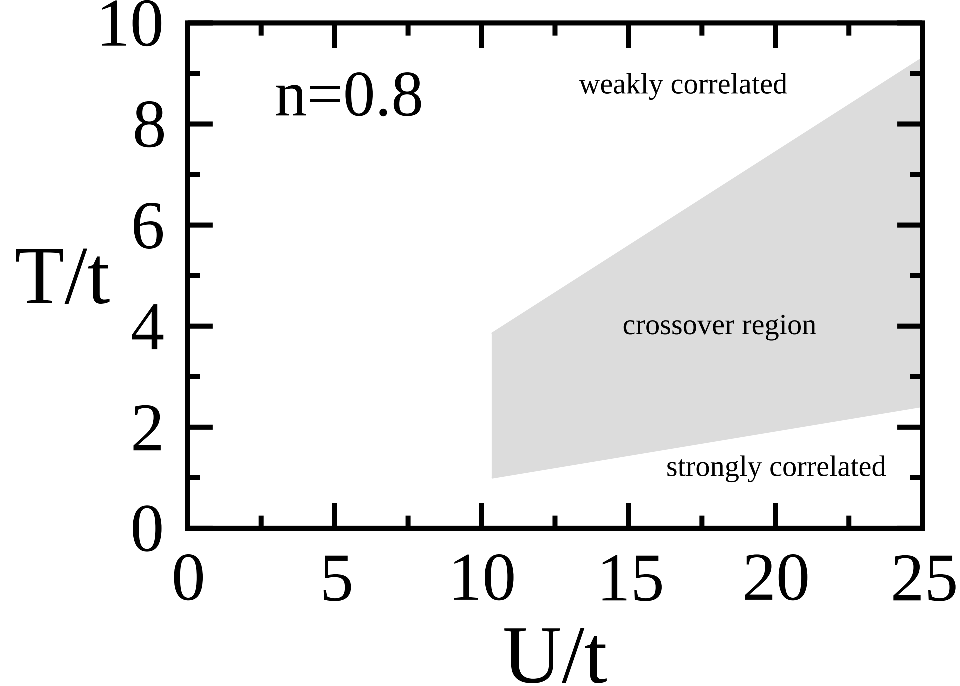
- The positive U Hubbard model also has a crossover

$$\lim_{\beta U \to 0} S = 2\left[-\frac{n}{2}\log\left(\frac{n}{2}\right) - \left(1-\frac{n}{2}\right)\log\left(1-\frac{n}{2}\right)\right]$$



$$\lim_{\beta U \to +\infty} S = -n\log(n) - (1-n)\log(1-n) + n\log(2)$$



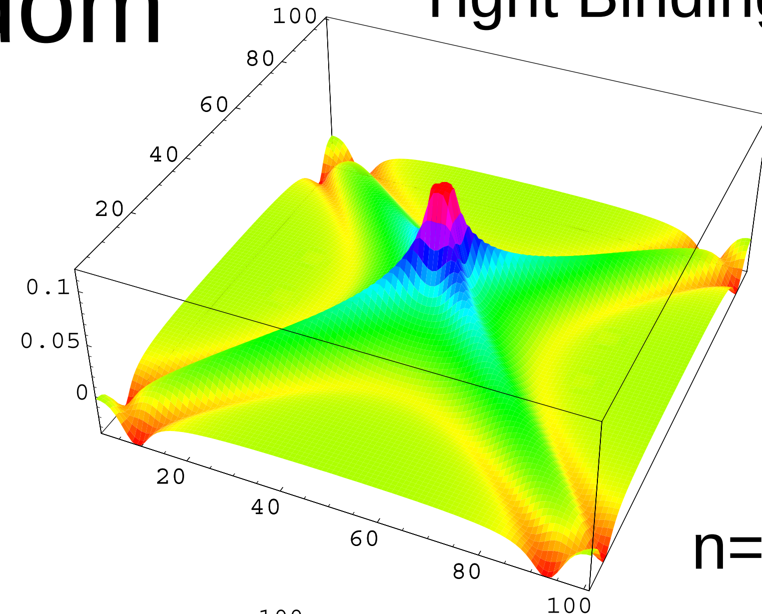


- For positive U the free energy is dominated by the entropy in the crossover temperature range
- The energy does not get smaller with larger U, unlike the negative U model.
- The low temperature degrees of freedom are determined by constrained entropy maximization – this is the origin of spin charge separation

Spin and Charge Degrees of Freedom

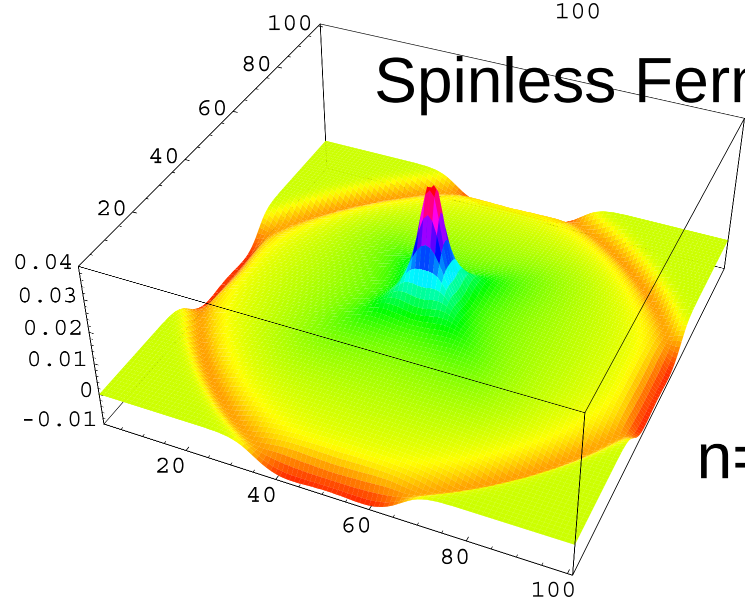
- Identify the degrees of freedom using the momentum dependence of the temperature derivative for correlation functions and compare to known non-interacting models
- Peak at Q = 0, negative derivative at Q = $2k_F$

Tight Binding



n=0.8

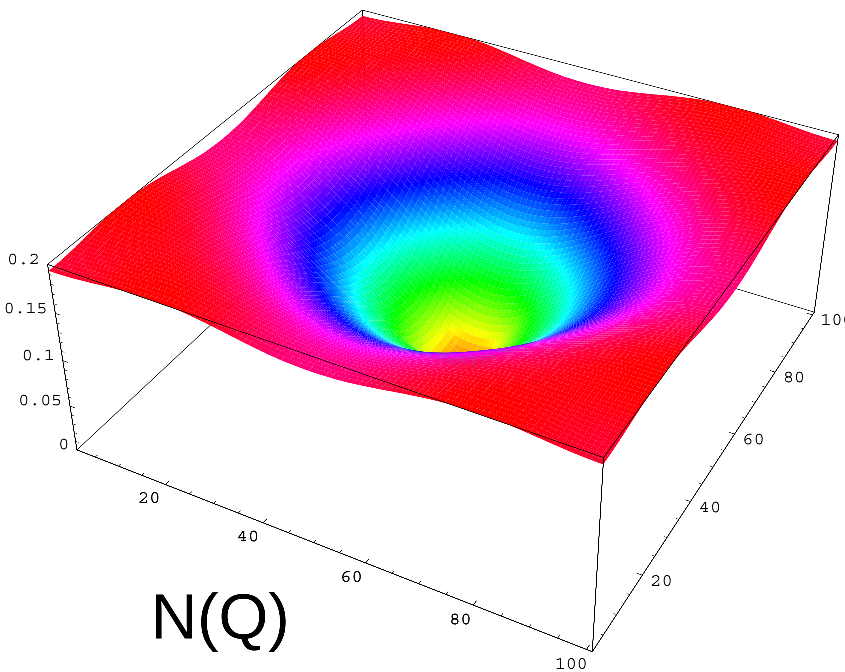
Spinless Fermions



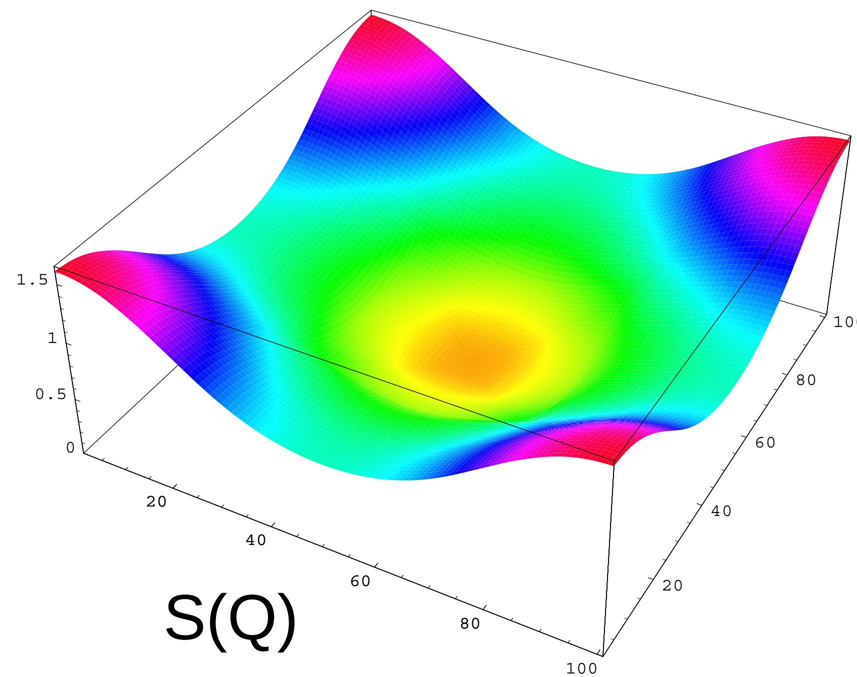
n=0.8

t-J Model Spin and Charge Correlation Functions

J/t = 0.4, n = 0.8,
T/J = 0.2



N(Q)



S(Q)

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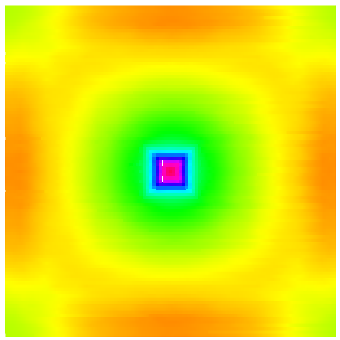
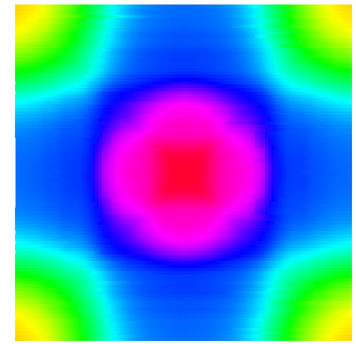
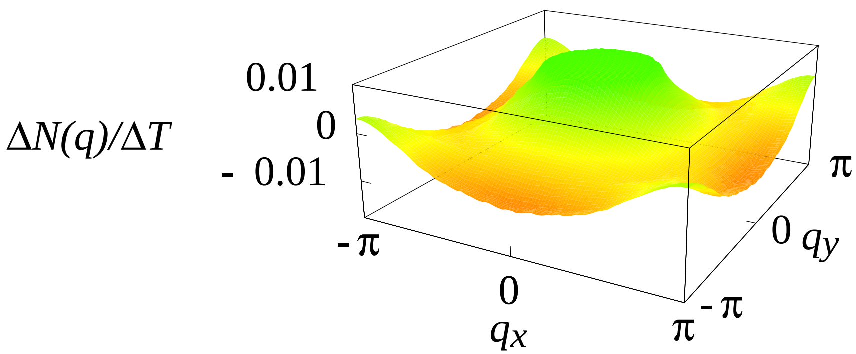
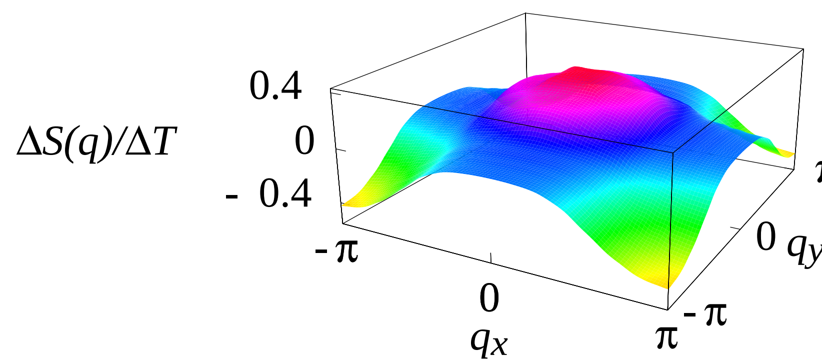
Temperature Derivatives of t-J Correlation Functions



T/J = 0.3







Charges act as hard core bosons with a coherence temperature of t, spins as spin-1/2 fermions with a coherence temperature of J/2. For J/t = 0.4 the ratio of the temperature scales is 5.

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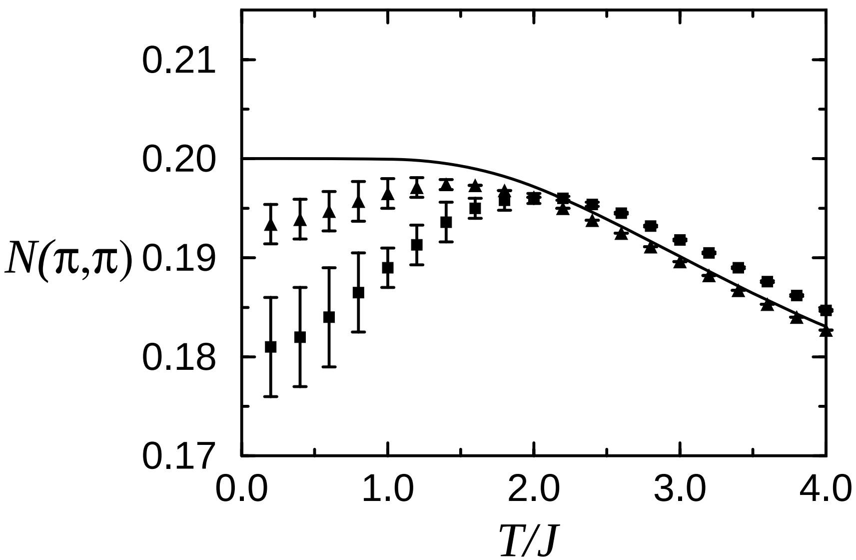
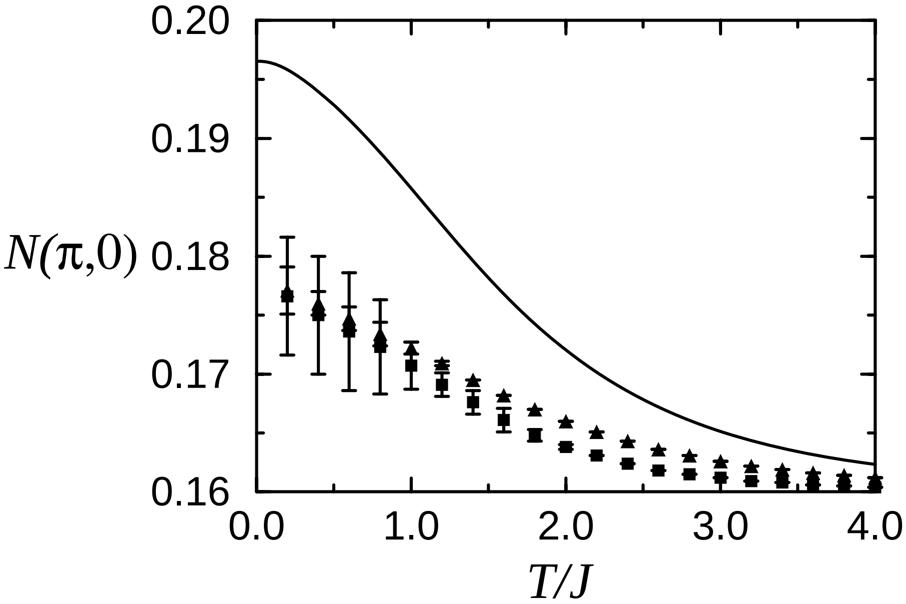
Temperature Dependence of Charge Correlation Function

Line=SF, Squares=HCB, Triangles=t-J Model



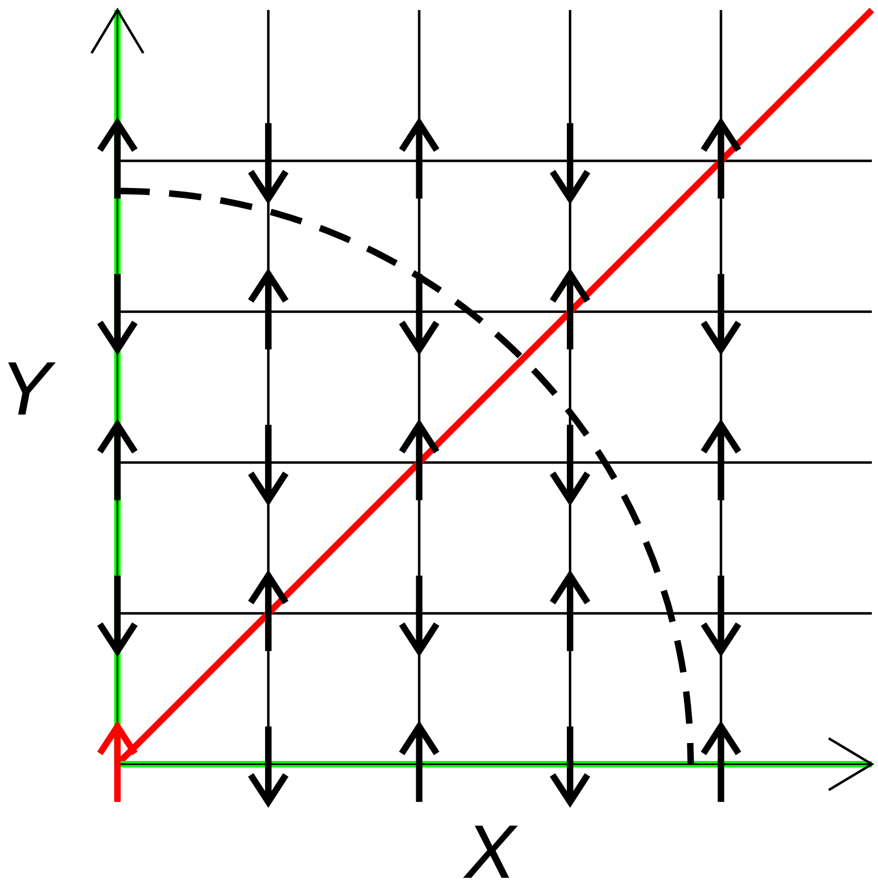


- The temperature scale for the charge degrees of freedom is T ~ 2.5J = t
- Below this temperature the charge degrees of freedom behave like hard core bosons

Fluctuations Leading to Strongly Correlated Superconductivity

- HCB will try to form a condensate $\langle b \rangle$ through fluctuations $\left\langle b_i^\dagger b_j \right\rangle$
- This condensate cannot form because the HCB are not fundamental particles
- Two boson fluctuations $\left\langle b_i^\dagger b_j^\dagger b_k b_l \right\rangle$ can grow because they can match up with the spin degrees of freedom to produce true electronic superconducting fluctuations

Symmetry of the Pair Fluctuations



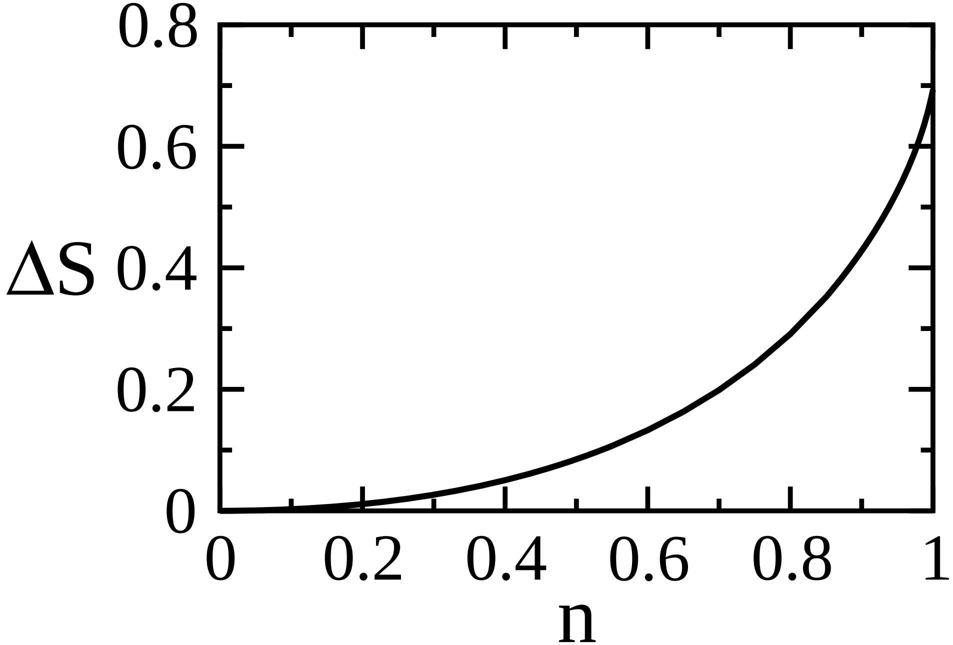
r = 3.8a

Symmetry	# Aligned Correctly	# Aligned Incorrectly
$d_{x^2-y^2}$	24	12
s	24	20
d_{xy}	16	16
p	18	20

- The spins, which for n = 0.8 have a coherence temperature of ~J/2, do not have sufficient energy to break up the existing boson pair fluctuations

- The coherent spins minimize the energy of the system by choosing the pair symmetry that best *avoids* the AF interaction

Density Range of Pair Fluctuations



- The entropy change in the crossover is strongly density dependent
- When the entropy change becomes too small energy gains from multi-site terms will dominate F = E – TS and spin charge separation will no longer be important, n ~ 0.45

$$\begin{aligned}\Delta S &= 2\left[-\frac{n}{2}\log\left(\frac{n}{2}\right)-\left(1-\frac{n}{2}\right)\log\left(1-\frac{n}{2}\right)\right] \\ &- [-n\log(n)-(1-n)\log(1-n)+n\log(2)]\end{aligned}$$

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Dependence of Pair Fluctuations on Dimension

- Excluded volume on a single site is the origin of spin-charge separation at high temperatures, so this happens in all dimensions
- BUT to produce pair fluctuations, a whole chain of conditions must be true
- In 1D HCB are identical to non-interacting SF, so there are no pair fluctuations
- In 3D Magnetic fluctuations are much stronger, leading to non-zero T_N and magnetism consuming most of the doping range where the entropy change (same in all dim.) is large
- 2D is where magnetism and superconductivity compete most favorably

Comparison to RVB

- RVB is based on spin-charge separation
- RVB also doesn't use an intermediate fluctuation to produce SC fluctuations
- Key difference: RVB uses the spin interaction to produce disordered spin singlets (spin liquid), while the idea presented here has the charge degrees of freedom produce pair fluctuations which the spin interaction then steers into d-wave electronic pair fluctuations
- Original RVB was s-wave

Conclusions

- The t-J model has $d_{x^2-y^2}$ pair fluctuations for realistic parameter choices for High-Tc
- Spin charge separation driven by constrained entropy maximization produces HCB and spin-1/2 degrees of freedom with a factor of ~ 5 difference in energy scales for model parameters most favorable to superconductivity
- The HCB drive the formation of pair fluctuations, while the spins choose the symmetry of the electronic pairs to best <u>compete</u> with the AF spin fluctuations present in the model