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SMR.627-15

MINIWORKSHOP ON
STRONGLY CORRELATED ELECTRON SYSTEMS

15 JUNE - 10 JULY 1992

"Dynamical Properties of Strongly Correlated Electrons"

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Dynamical Properties of Strongly Correlated Electrons.

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Florida State University

- High-Tc Superconductors

  i) $N(\omega)$, PES, IPES
  ii) ARPES, ARIPES
  iii) $\sigma(\omega)$

  one band Hubbard and t-J models.

  iv) Superconductivity?

  No indications in Hubbard model.
  Results for 2D t-J model at $\langle n \rangle = 1/2$ suggest superconductivity near phase separation!

- C_{60}

  QMC study at half-filling using Hubbard model.

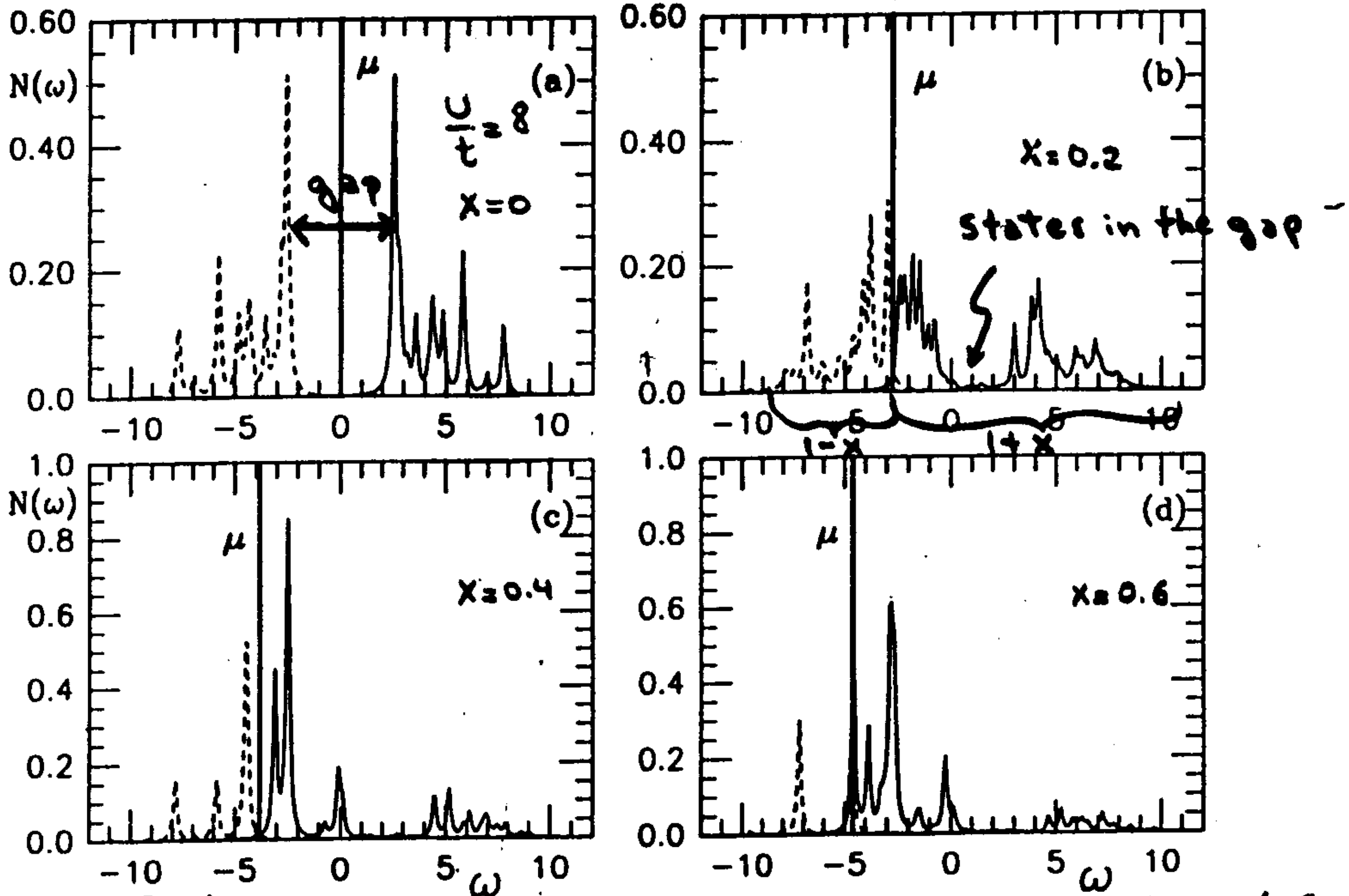
How can we study the Hubbard model in strong coupling?

<u>One way</u>: numerical studies

<u>Exact diagonalization</u> (Lanczos)	<u>Q. Monte Carlo</u>
Solve exactly a small cluster (4x4)	Larger lattices possible (8x8) (16x16)
• $T=0$	• $T \neq 0$
• Exact	• Stat. errors
• No "sign" problems	• "sign" problems
• Dynamics easy	• Dynamics difficult

Review:
(See Int. J. Mod. Phys. <u>B5</u>, 77, 1991.)

<u>Other ways</u>: { mean-field
variational
...



E.D., A.Moreo, F.Ortolani, J.Riera, D.Scalapino, PRL 67, 1918 (1991).

FIG. 3. Same as Fig. 2 with $U/t=8$. (10 and 16 sites clusters give similar results)

ole doping are to remove spectral weight from both the upper and lower Hubbard bands and to create additional density of states in the gap beginning at the edge of the lower Hubbard band. Results for further dopings are shown in Figs. 2(c) and 2(d). With this additional dop-

slope is *larger* than one (at small x) and increases when U/t is reduced, at least for U/t large where a genuine gap exists in the IPES spectrum.

Thus we find, as seen in PES experiments [2], that doping a half-filled Hubbard cluster does not simply produce a rigid shift of the density of states relative to the

3

μ moves across the gap when going from holes to electrons doping

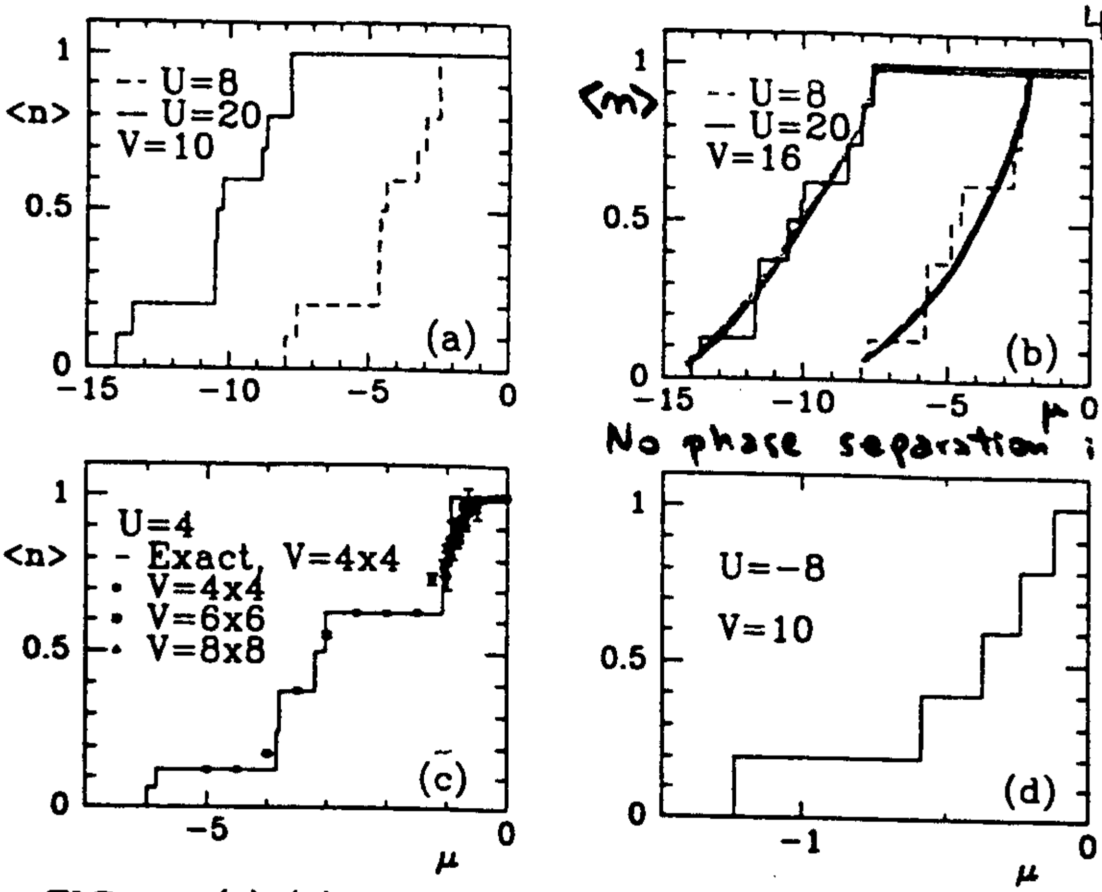


FIG. 1. (a) $\langle n\rangle$ vs μ at zero temperature for the ten-site Hubbard cluster with $U/t=20$ (continuous line) and $U/t=8$ (dashed line) using Lanczos techniques; (b) same as (a) for a sixteen-site cluster; (c) $\langle n\rangle$ vs μ at $U=4$ $(t=1)$. The continuous line is the Lanczos result for the sixteen-site cluster. Solid squares denote Monte Carlo results on a 4×4 lattice at temperature $T=t/12$, while the open squares and the solid triangles are Monte Carlo results for the 6×6 and 8×8 clusters, respectively, with $T=t/8$; (d) $\langle n\rangle$ vs μ at zero temperature for the ten-site Hubbard cluster with $U/t=-8$ using Lanczos techniques.

particle-hole transformation, to the statement that the magnetic spin susceptibility of the positive-U Hubbard model at half filling remains finite as the temperature T goes to zero. Likewise the result that $\partial\langle n\rangle/\partial\mu|_{\mu=0}$ van-

ishes for the
the vanishing
negative-U H
chemical pote
slowly move a
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In order to
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$N_s^{(+)}(\omega)=\frac{1}{\ldots}$

$N_s^{(-)}(\omega)=\ldots$

Here $N_s^{(+)}(\omega$
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of states for
ground state
lattice sites,
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ground state
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$N\pm1$ electr
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ω for $U/t=$
Fig. 1) is sho
half filling (
the lower H
are removed
Comparing I

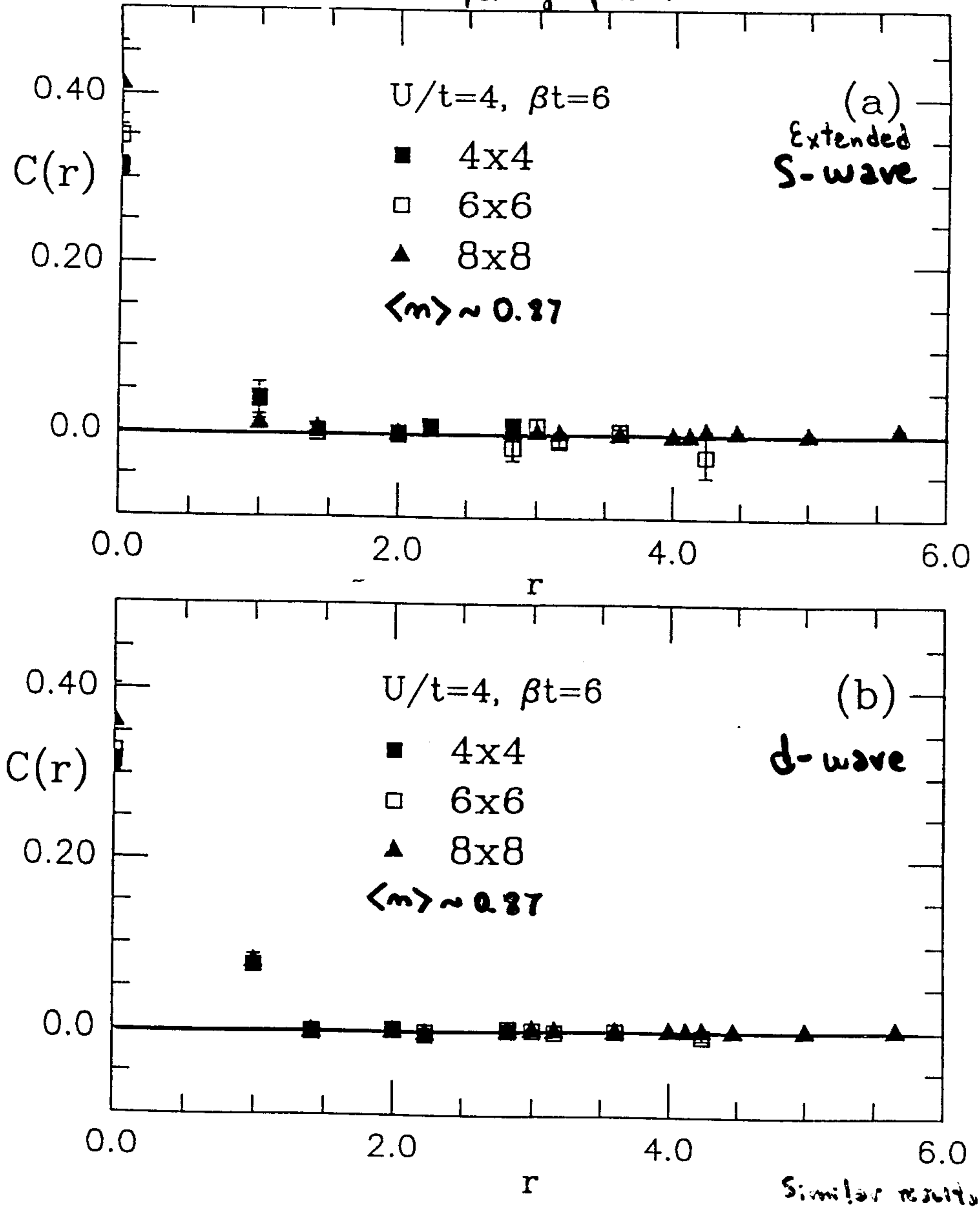
... thus far ...

		Exper.	Theory	
$N(\omega)$	New states in gap	yes	yes	
	μ changes when going from hole to e^- doping	yes (x-ray) (C. Chen et al. PRL <u>66</u>, 104) no (PES) (J. Allen et al., PRL <u>64</u>, 595)	yes	
ARPES	quasiparticle	maybe	yes	
	$\frac{m^*}{m} \sim 2-3$	yes (Arko et al.)	yes	
Raman	half-filling	good agreement		
	doping	?		
$\sigma(\omega)$		good agreement mid-IR, N_{eff}, ...		← See A. Tikofsky, Laughlin + Zou Q15 (anyon superc. state)
$S(\vec{q})$	shift of AF peak from (π,π) to $(0,\pi)$	yes	yes	← A. Moreo et al., PRB <u>41</u>, 2313
Superconductivity		yes	?	

$C(r) = \langle \Delta(0)\, \Delta^{\dagger}(r) \rangle$

↑ pairing operator

(A. Moreo, ~~to appear~~ in PRB) published



No superconductivity!

Similar results using other methods and ... Hubbard

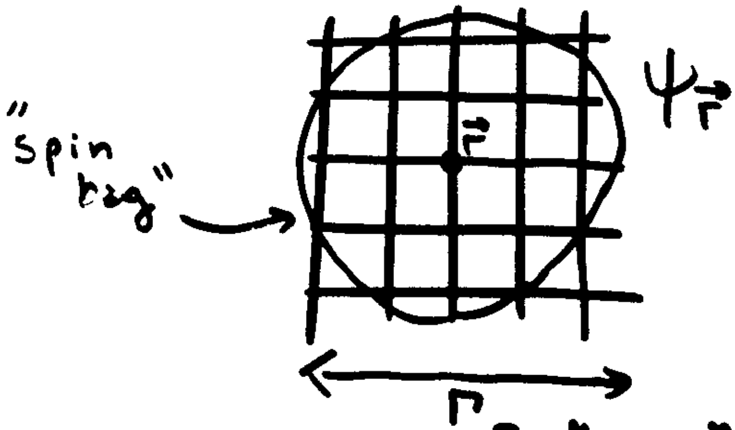
Why we don't see superconductivity in the Hubbard model?

- $J = \frac{4t^2}{U} \sim 0.1\,eV \sim 1000\,K$
  $t \sim 0.43\,eV \sim 4300\,K$
  $T_c \sim 100K$ More difficult
- temperature in MC too high?
- Hubbard model doesn't superconduct
- we are not using the best operators

Intuitive idea:

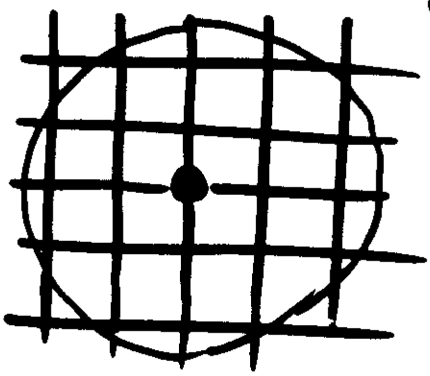
(E.D. + J.R. Schrieffer) PRB 43, 8705 (1991);
See also: M. Boninsegni + E. Manousakis, PRB 43, 10353

$$\psi_{\vec{q}} = \sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}}\,\psi_{\vec{r}}\ , \qquad H\psi_{\vec{q}} = E\,\psi_{\vec{q}}$$



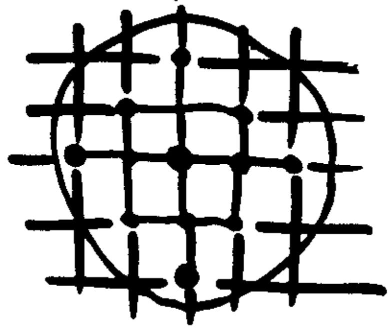
Γ "size" of quasiparticle

local "antenna" $c^{+}_{\vec{r}}$



$Z \ll 1$

extended "antenna" $\tilde{c}^{+}_{\vec{p}} = c^{+}_{\vec{r}} + \alpha \sum_{\mu} c^{+}_{\vec{r}+\mu}\, c_{\vec{r}}\, c^{+}_{\vec{r}} + \ldots$



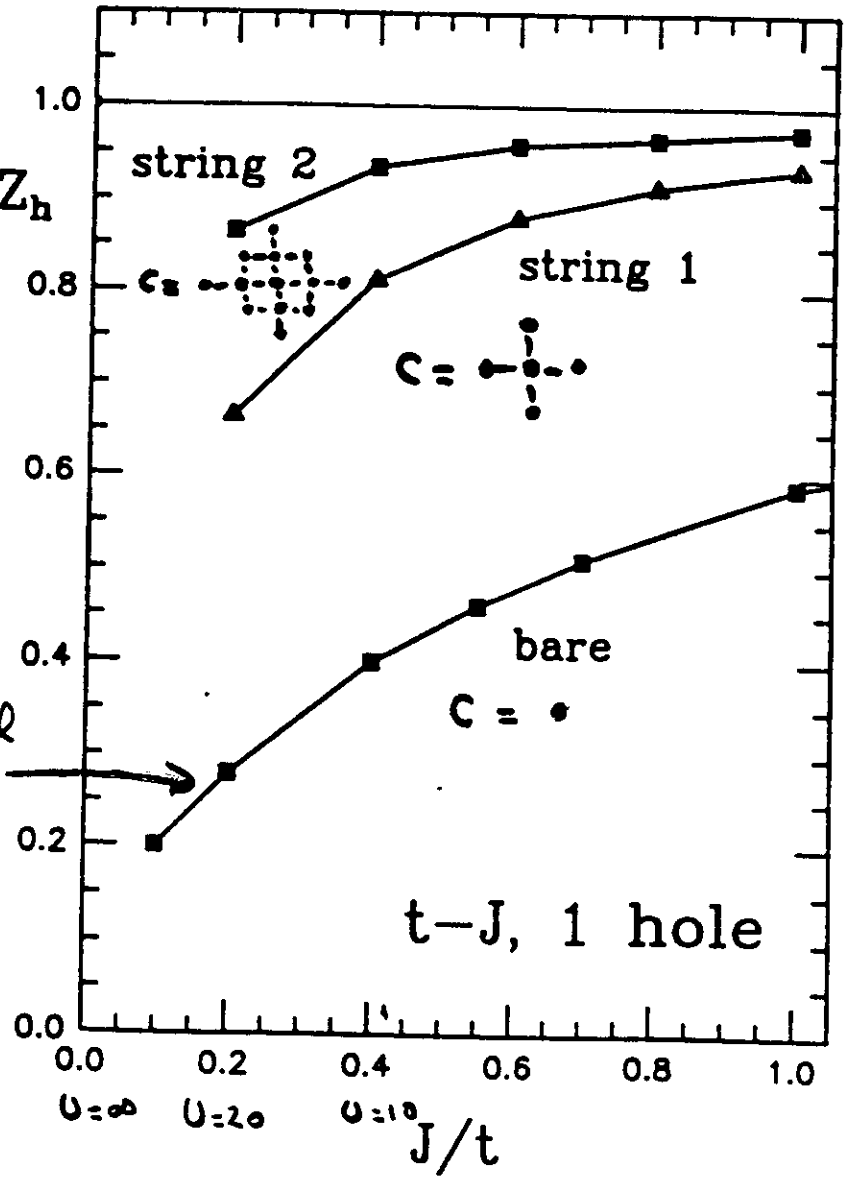
$Z \simeq 1$

This concept is valid for any H and any operator involving quasiparticles. It filters out higher energy states.

Preliminary numerical results show that the idea works! ($Z \approx 1$)

where H_t (H_{Heis}) is the hopping (exchange) inter
the t-J model and β is another constant. The con
guarantees that to this order the spinlike ex
relevant for the dressing of the hole are creat
neighborhood. The hopping term moves the hole

t-J model
1 hole



Note: $Z \neq 0$ in t-J model
$Z \sim J^{1/2}$ at small J.

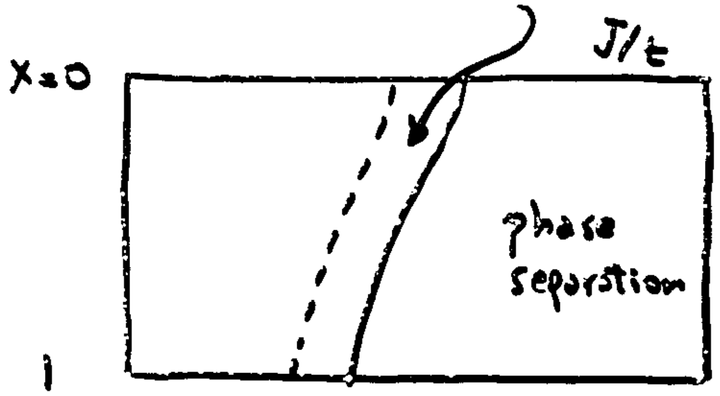
Confirmed by
D. Poilblanc (N=26)

(In Hubbard model
Sorella claims $Z \to 0$)

FIG. 1. Z_h of one hole as a function of J/t for the t
on a 4×4 lattice. Results are shown using the bare f
operator (■), strings of length 1 (△), and strings of len
citations (■) in the "dressed" fermionic operator.

- t-J model is more promising

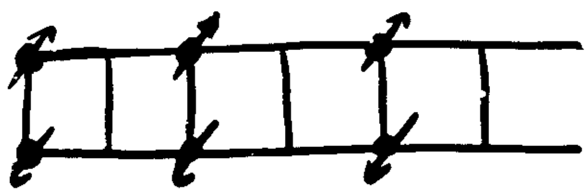
– In 1D there is a region where supercond. correlations dominate



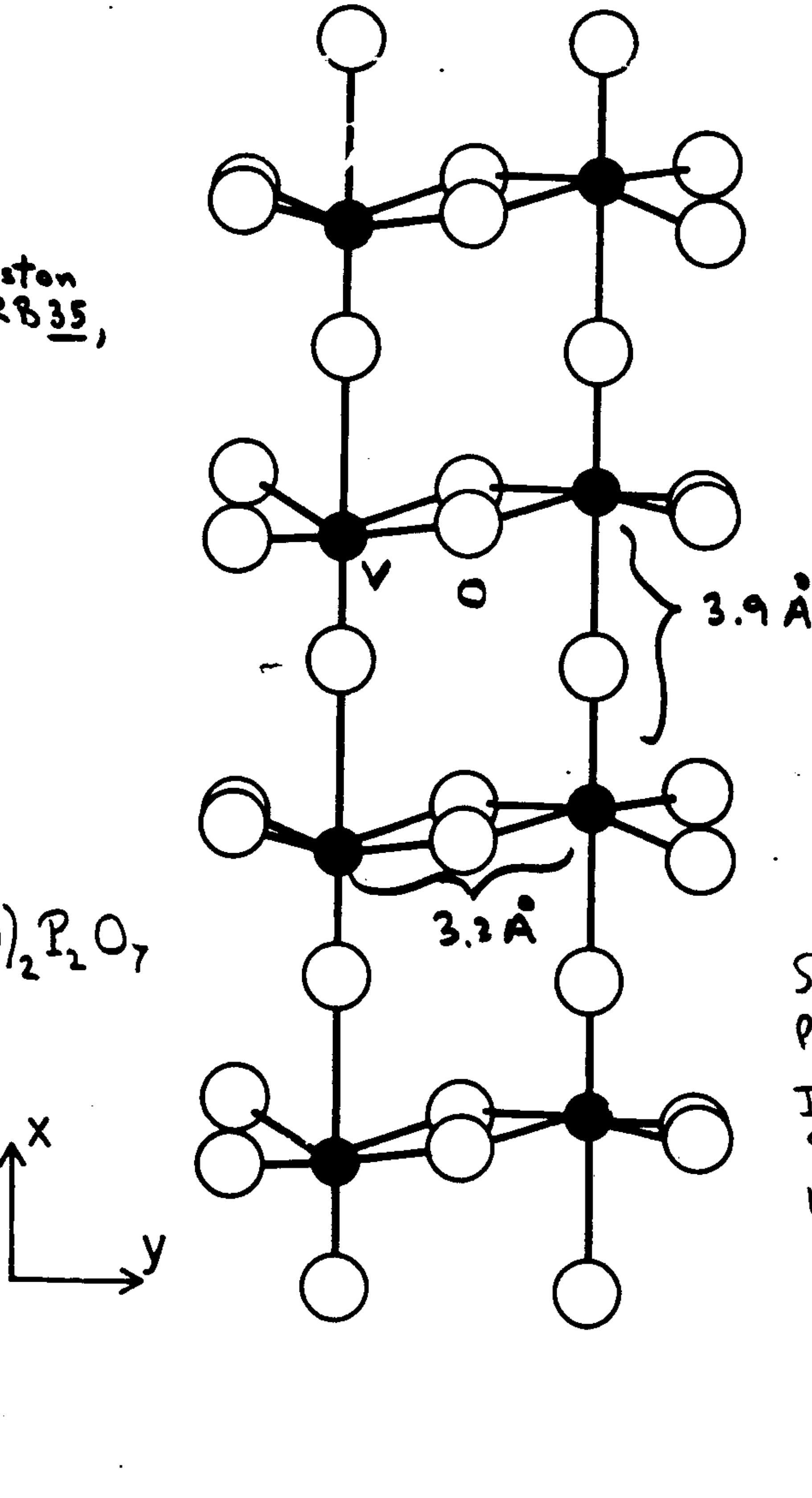
See M. Ogata et al., PRL 66 2388 (91)

– In 2D a study of the spectrum of finite clusters suggest similar results. See A. Moreo, PRB

– In "ladders" and $J/t > 1$, supercondu. dominates. (dimerization process)



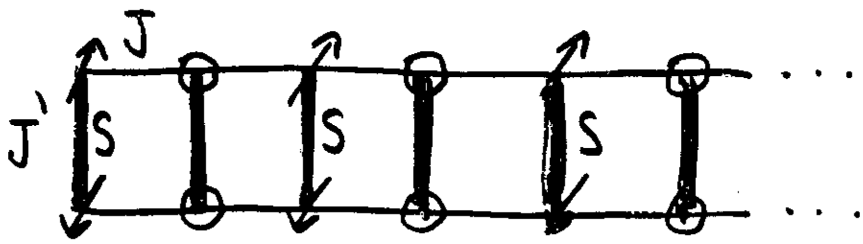
D.C. Johnston et al., PRB 35, 219 (87)



$(VO)_2P_2O_7$

See E.D. et al., PRB, ~~March 92~~ 45, 5744, Imada, J. Phys. Soc. Jpn. 60, 1877 (91)

$\langle n \rangle = 1/2$

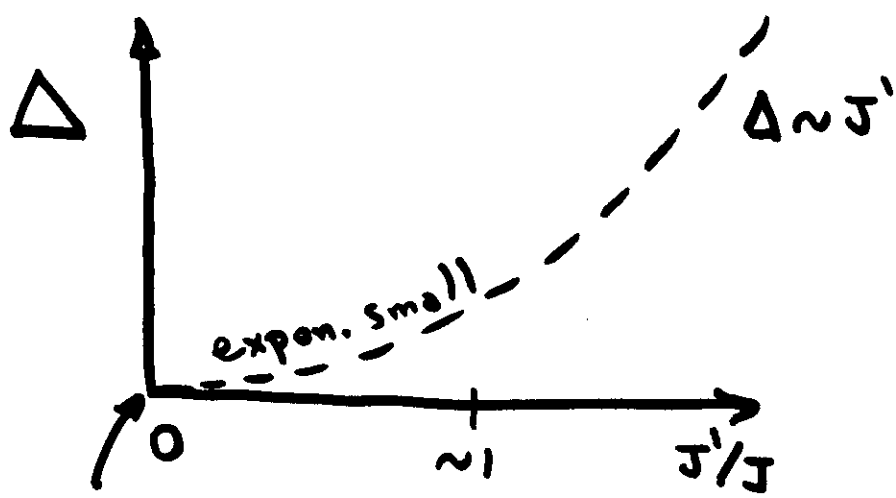


if $J' \gg J, t \rightarrow$ superconductivity
(as in $U<0$ Hubbard)

Numerical results suggest that
for $J' \sim J$ we can still have supercond.

No phonons, purely electronic.

Recent QMC results at $\langle n \rangle = 1$ suggest: (Barnes et al.)



– t-J-V model $\left(V\sum_{\langle ij\rangle} n_i n_j\right)$ ← See also Kovarik + Barnes

1D, $\langle n\rangle = 1/2$

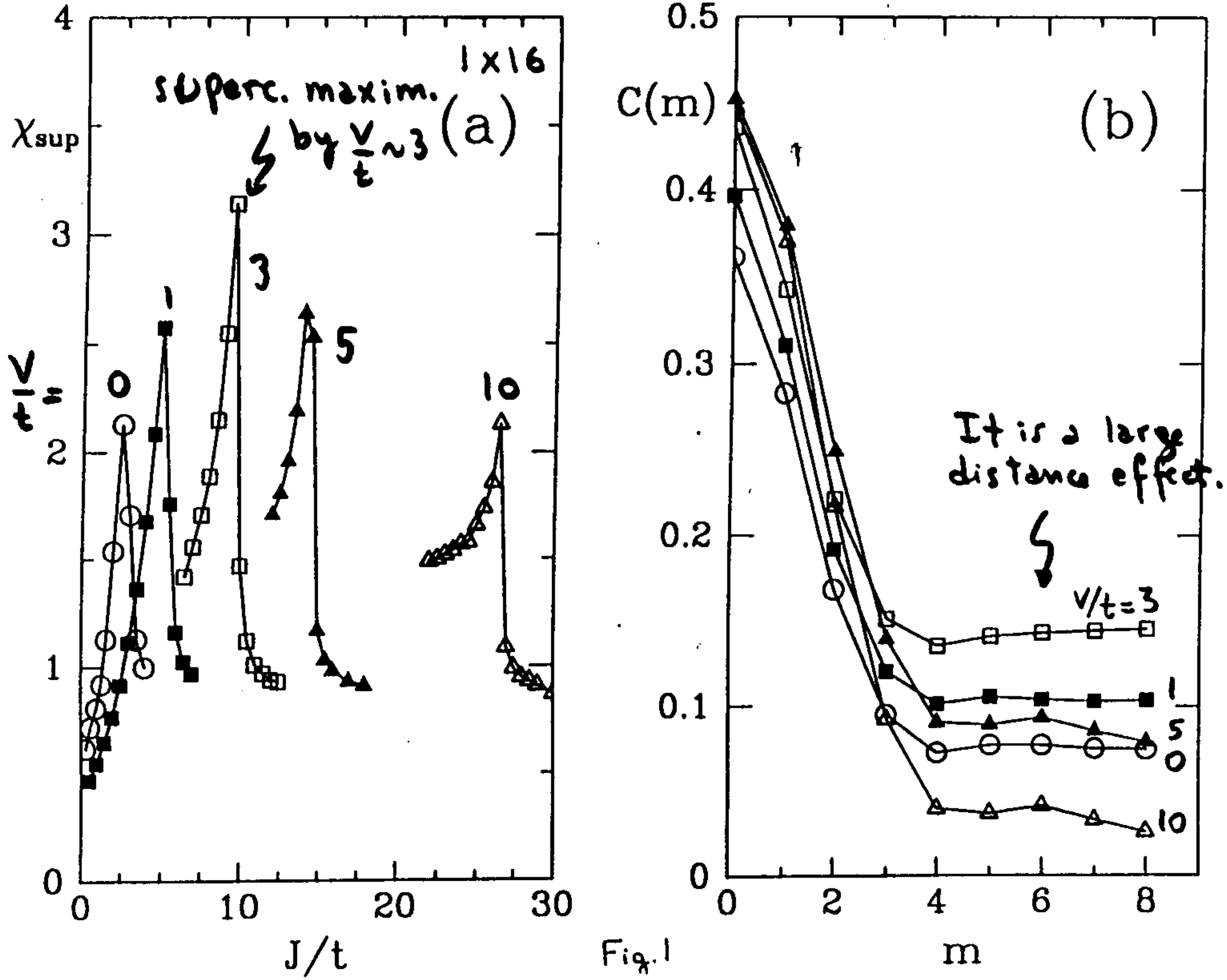


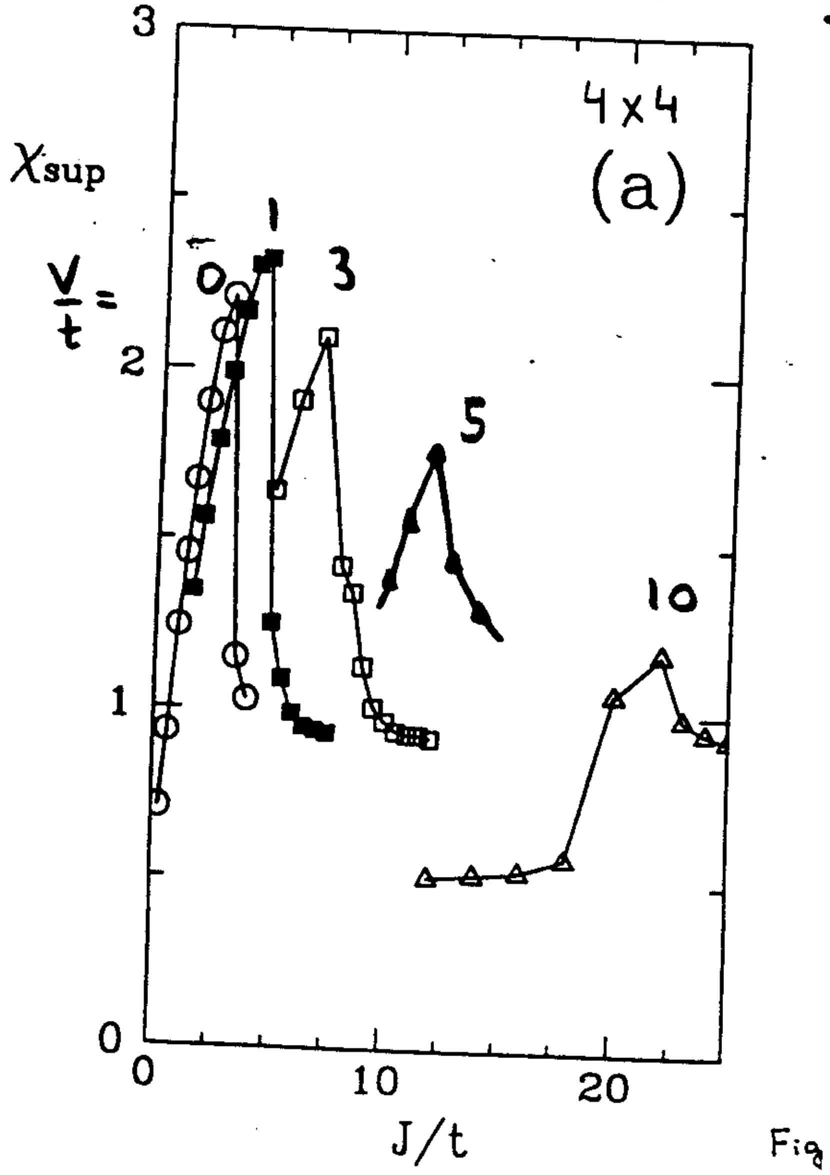
Fig. 1

E.D. + Jose Riera, preprint

2D, $\langle n \rangle = 1/2$

Very similar to 1D.

There is a spin-gap.



The same quantity near half-filling is flat. So we may have been looking at the wrong doping!

Fig

Why the superconducting correlations are enhanced in 2D near $\langle n \rangle = 1/2$?

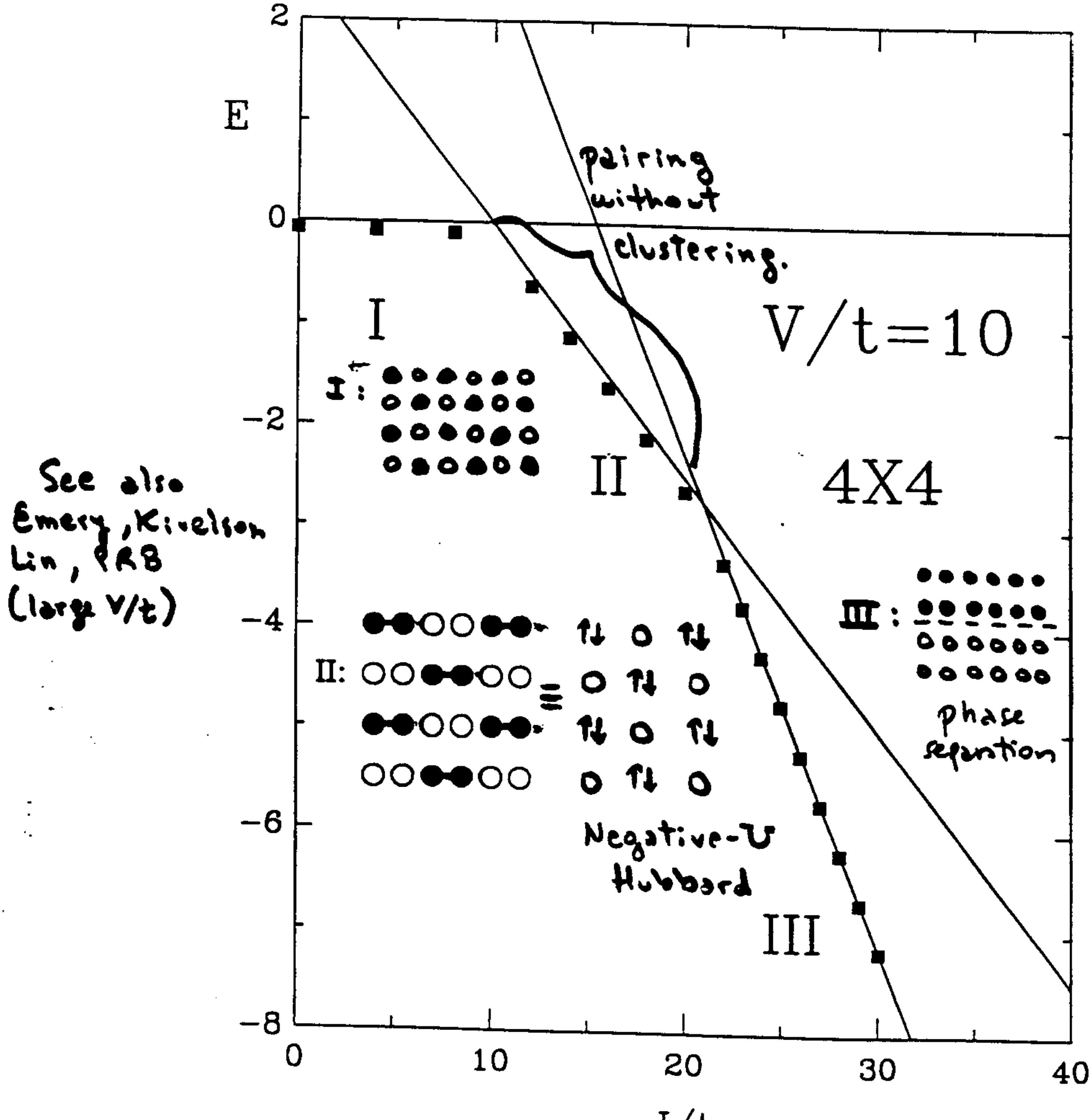
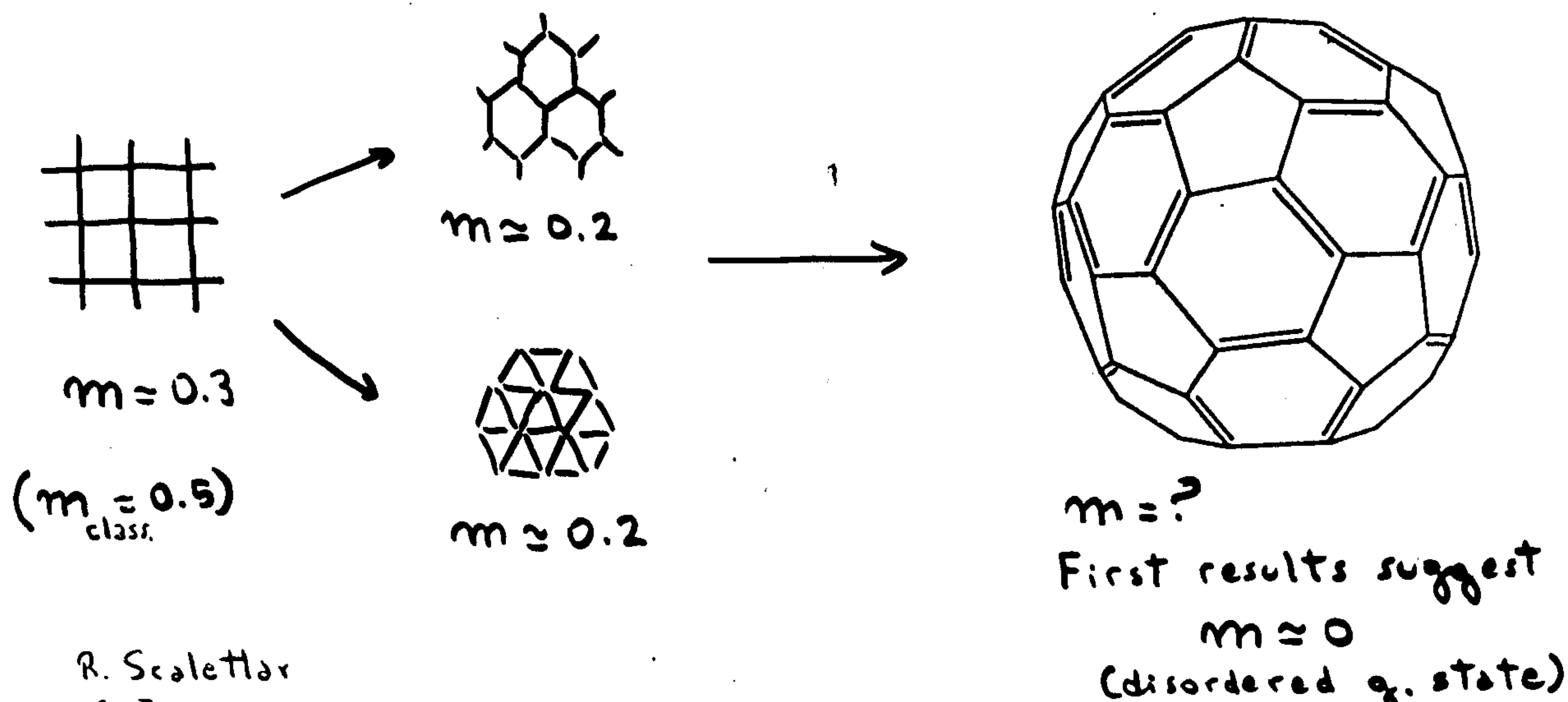


Fig. 4

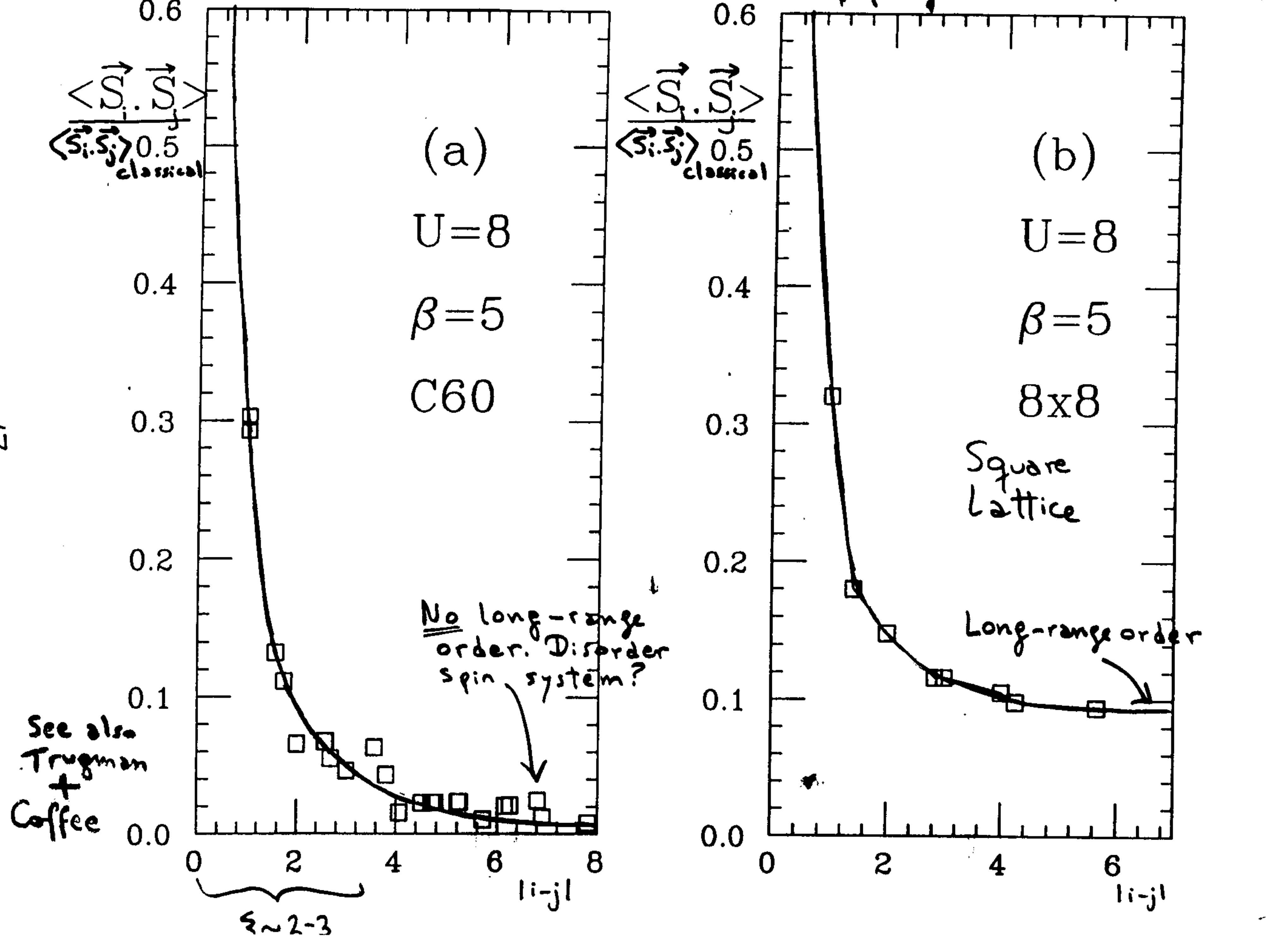
C_{60} :

Heisenberg model on a ball
(spin 1/2)



R. Scalettar
T. Jolicoeur
H. Monien
E. D., ~~in preparation~~. sent to PRL.

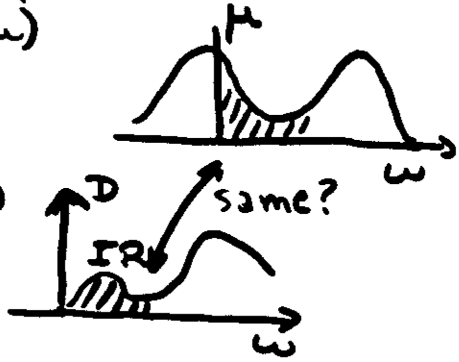
Hubbard model at half-filling. (Chakravarty + Kivelson)



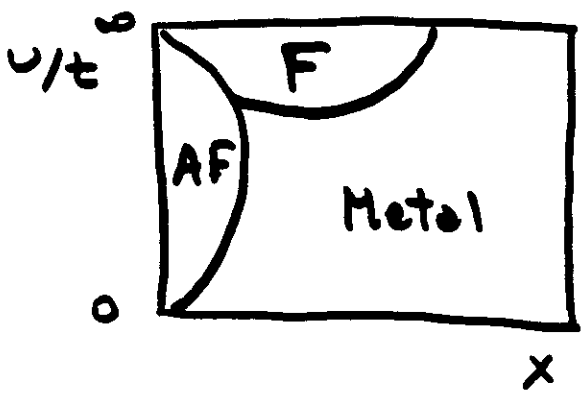
Conclusions

1) Some "unusual" normal state properties may be explained by Hubbard model.

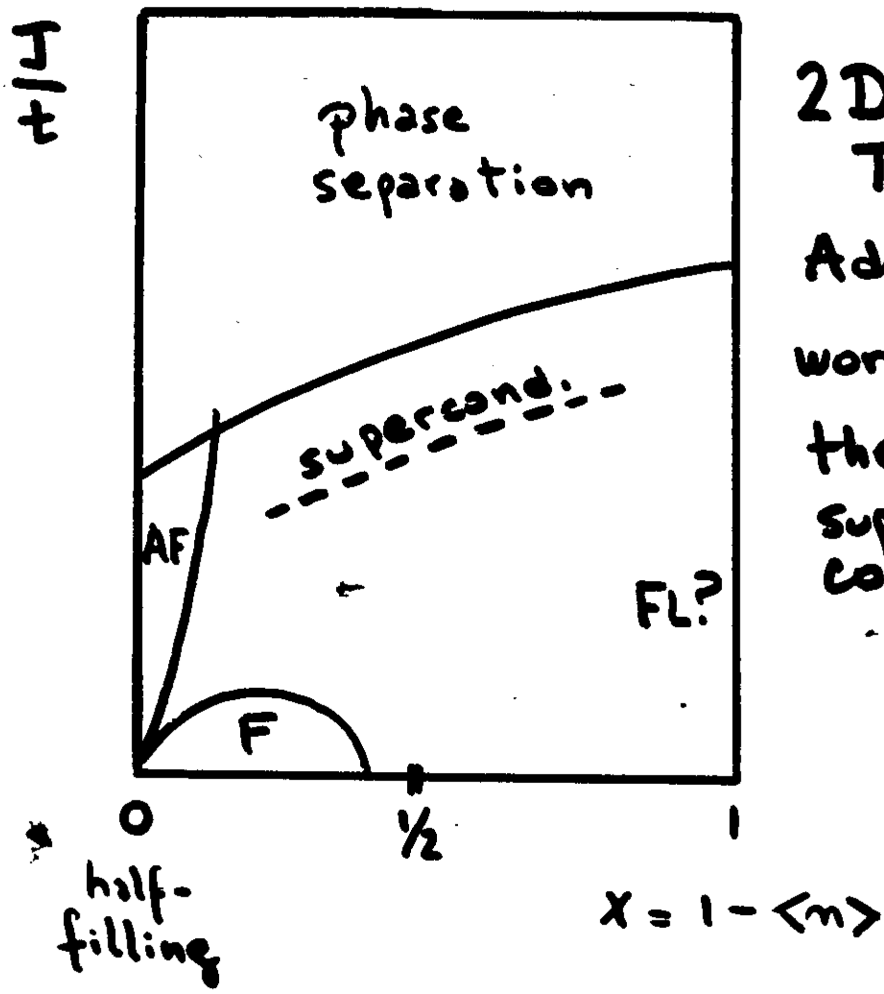
   a) quick loss of AF with x
   b) $S(q)$ IC
   c) $N(\omega)$
   d) $\sigma(\omega)$



2) Superconductivity in Hubbard model?
Either the model has to be "modified" or new quasiparticle operators will solve the problem.



3) The t-J model seems to have more structure:



2D t-J
T=0

Adding $\frac{V}{t}$ and working at $\langle n \rangle = \frac{1}{2}$ there are strong superconducting correlations.

—o—