The Superconducting Transition Temperature Tc for some Basic Models

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UCSB

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Phys. Rev. 134, A1416 - A1424 (1964)

Possibility of Synthesizing an Organic Superconductor

W. A. Little

Department of Physics, Stanford University, Stanford, California

Received 13 November 1963; revised 27 January 1964

London's idea that superconductivity might occur in organic macromolecules is examined in the light of the BCS theory of superconductivity. It is shown that the criterion for the occurrance of such a state can be met in certain organic polymers. A particular example is considered in detail. From a realistic estimation of the matrix elements and density of states in this polymer it is concluded that superconductivity should occur even at temperatures well above room temperature. The physical reason for this remarkable high transition temperature is discussed. It is shown further that the superconducting state of these polymers should be distinguished by certain unique chemical properties which could have considerable biological significance.

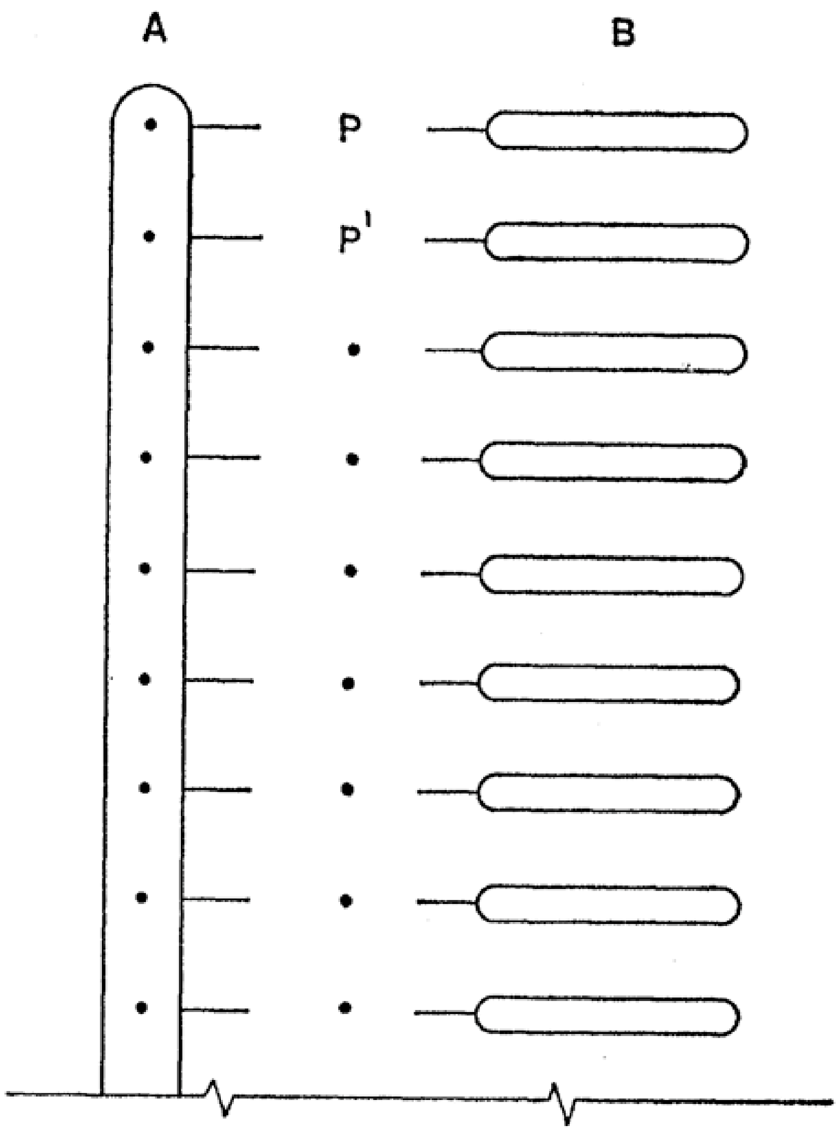


FIG. 1. Proposed model of a superconducting organic molecule. The molecule A is a long unsaturated polyene chain called the "spine." The molecules B are side chains attached to the spine at points P, P′, · · ·.

Some problems and questions raised regarding Little's 1964 work:

Fluctuations
Competition with CDW and Peierls phases
Strength of coupling g
Retardation
Structure and microstructure

What can we say about the questions that Little's work , the heavy fermions , the cuprates and MgB2 have raised about achieving room temperature superconductivity?

Results for some simple model systems?

The negative U Hubbard model

The Holstein Model on a 2D lattice

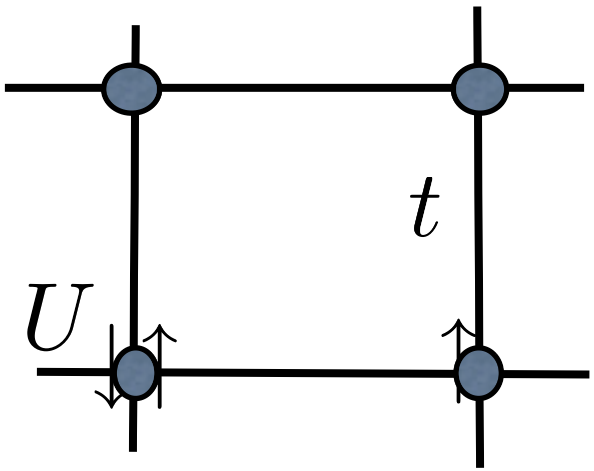
The positive U Hubbard model on a 2D lattice

The 2-leg Hubbard ladder

Conclusions

Competition and strength of interaction

The Hubbard Model



$$H = -t \sum_{<i,j>\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

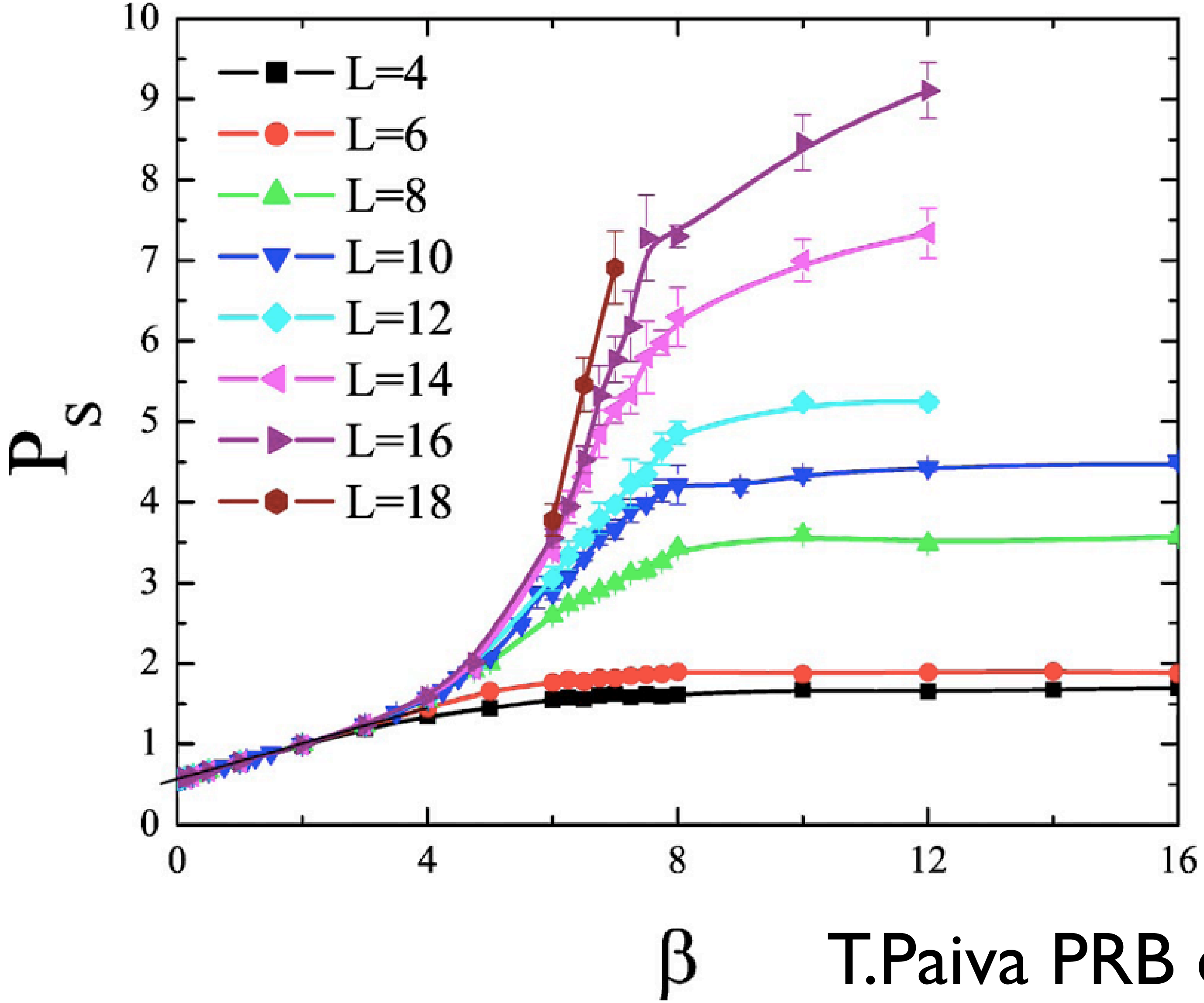
It depends upon only two parameters
U/t and the site filling <n>=1-x

The pair-field susceptibility

$$P_s(T) = \int_0^\beta d\tau < \Delta(\tau)\Delta^\dagger(0) >$$

with $\quad \Delta^\dagger = \frac{1}{\sqrt{N}} \Sigma_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$

Pairfield Susceptibility <n>=0.87 U=-4t



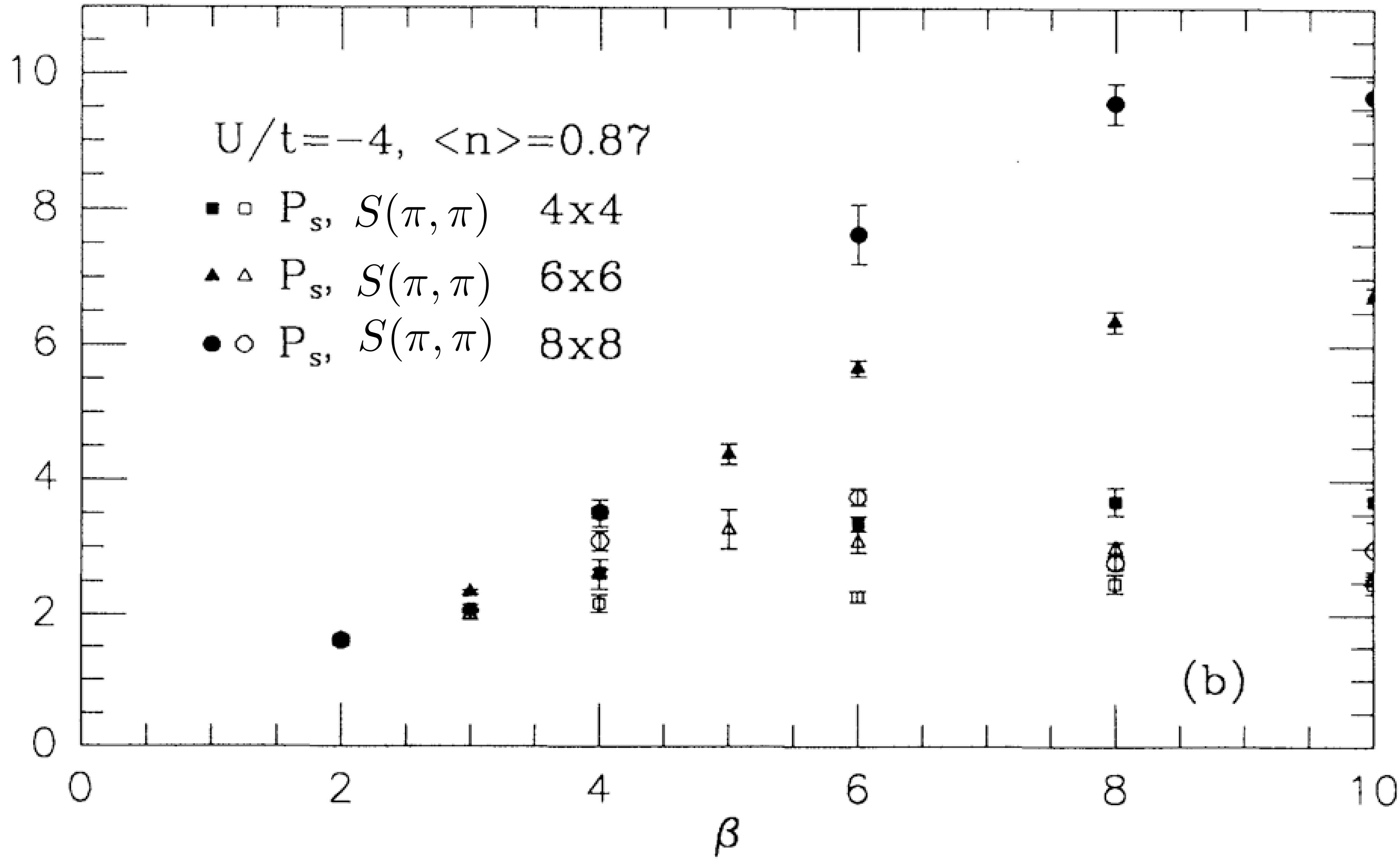
T.Paiva PRB et al 2004

The charge structure factor

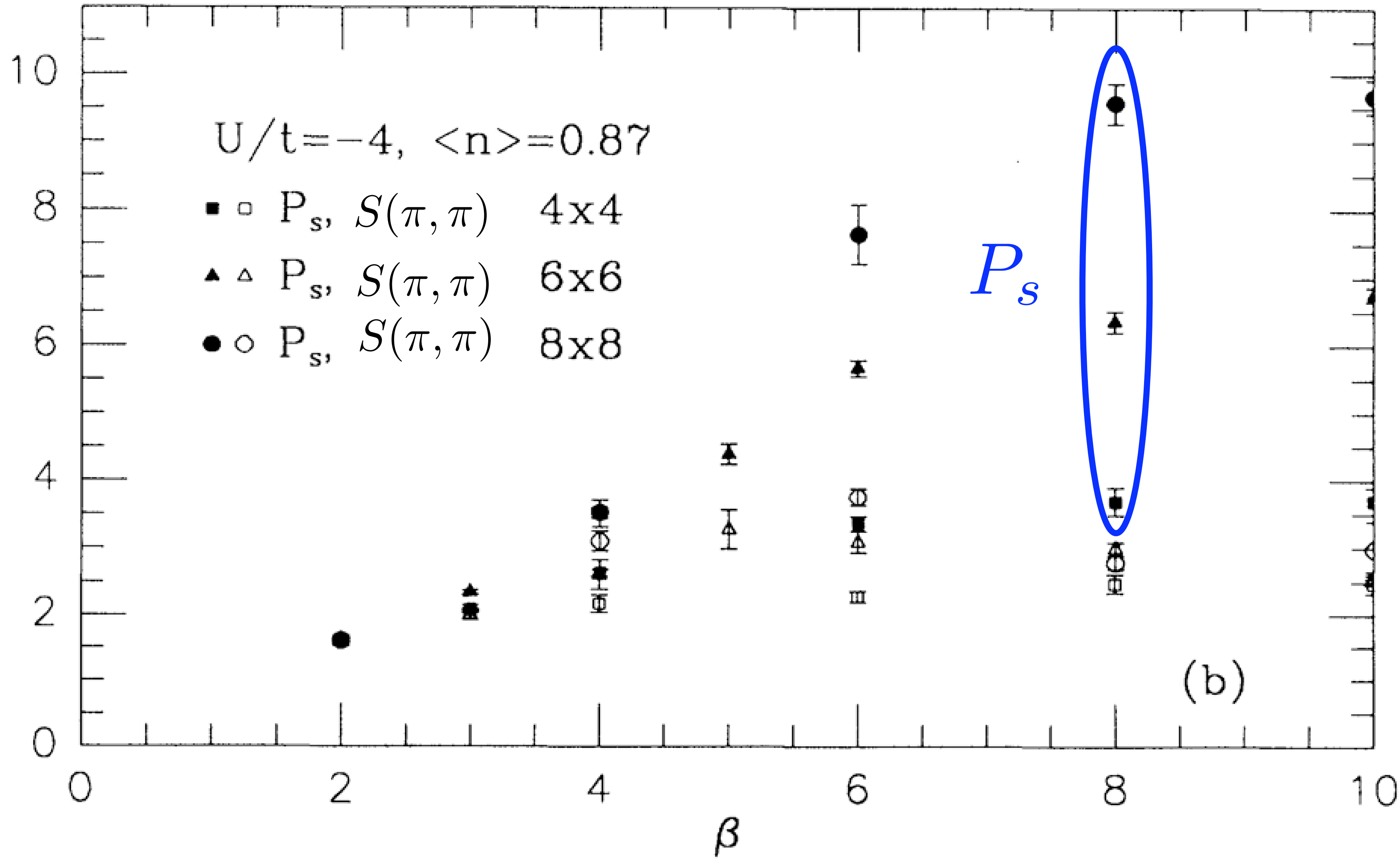
$$\mathsf{S}(q) = \frac{1}{N} < \rho_q \rho_q^\dagger >$$

with

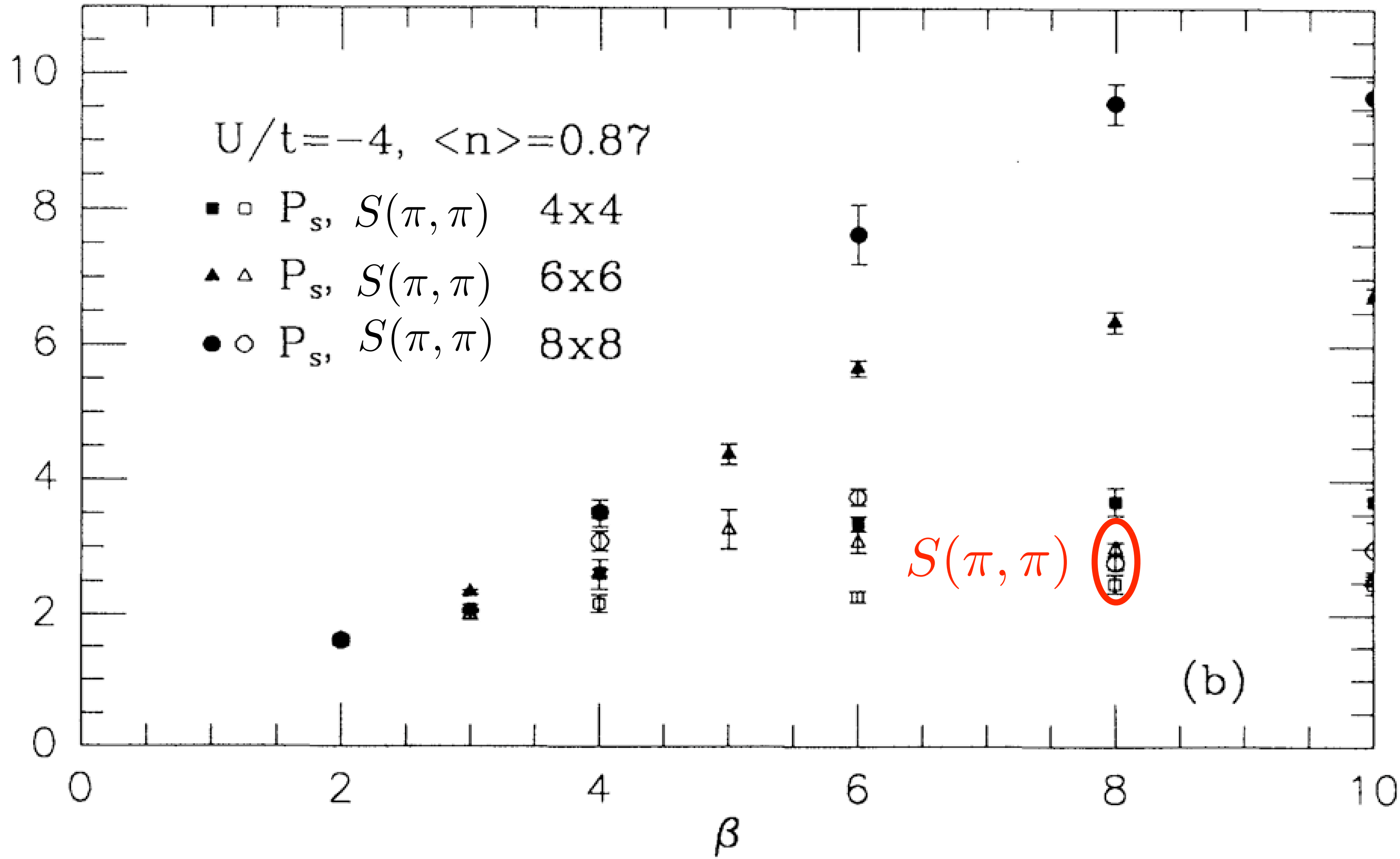
$$\rho_q^\dagger = \sum_{l,\sigma} e^{i\mathbf{q.l}} c_{l\sigma}^\dagger c_{l\sigma}$$



Moreo and Scalapino PRB 1991

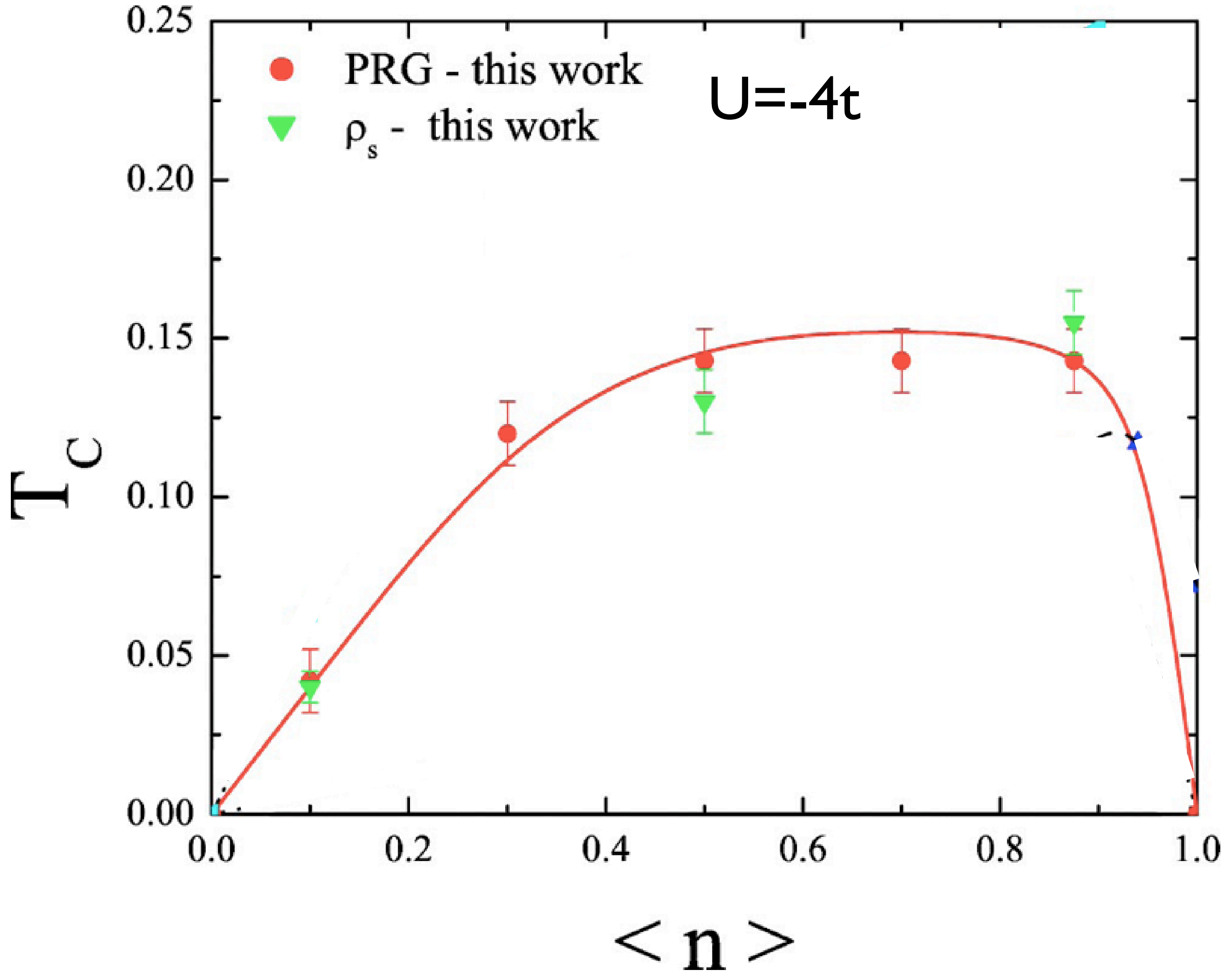


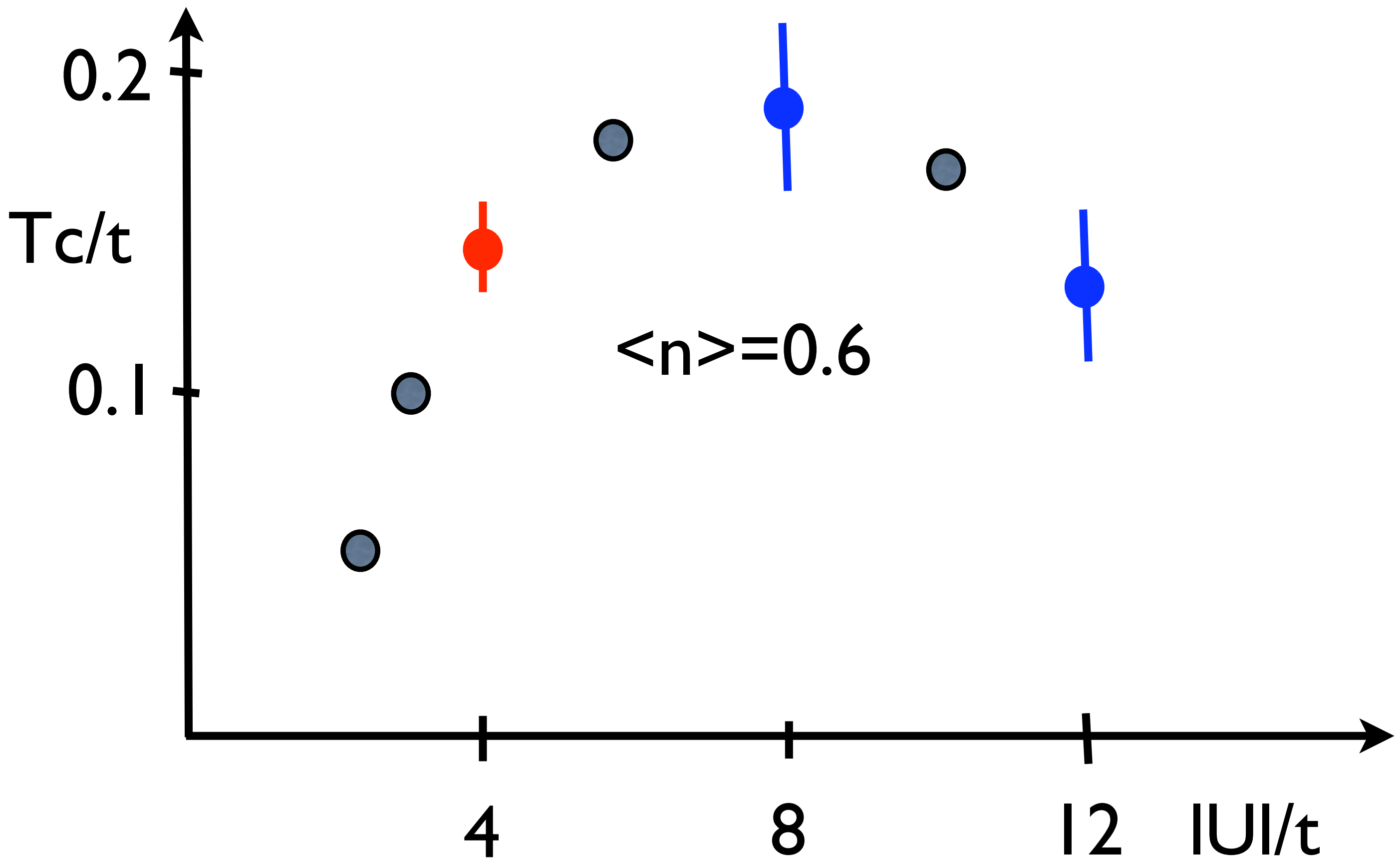
U/t=−4, <n>=0.87
P_s, S(π,π) 4x4
P_s, S(π,π) 6x6
P_s, S(π,π) 8x8
P_s
(b)
β
0
2
4
6
8
10



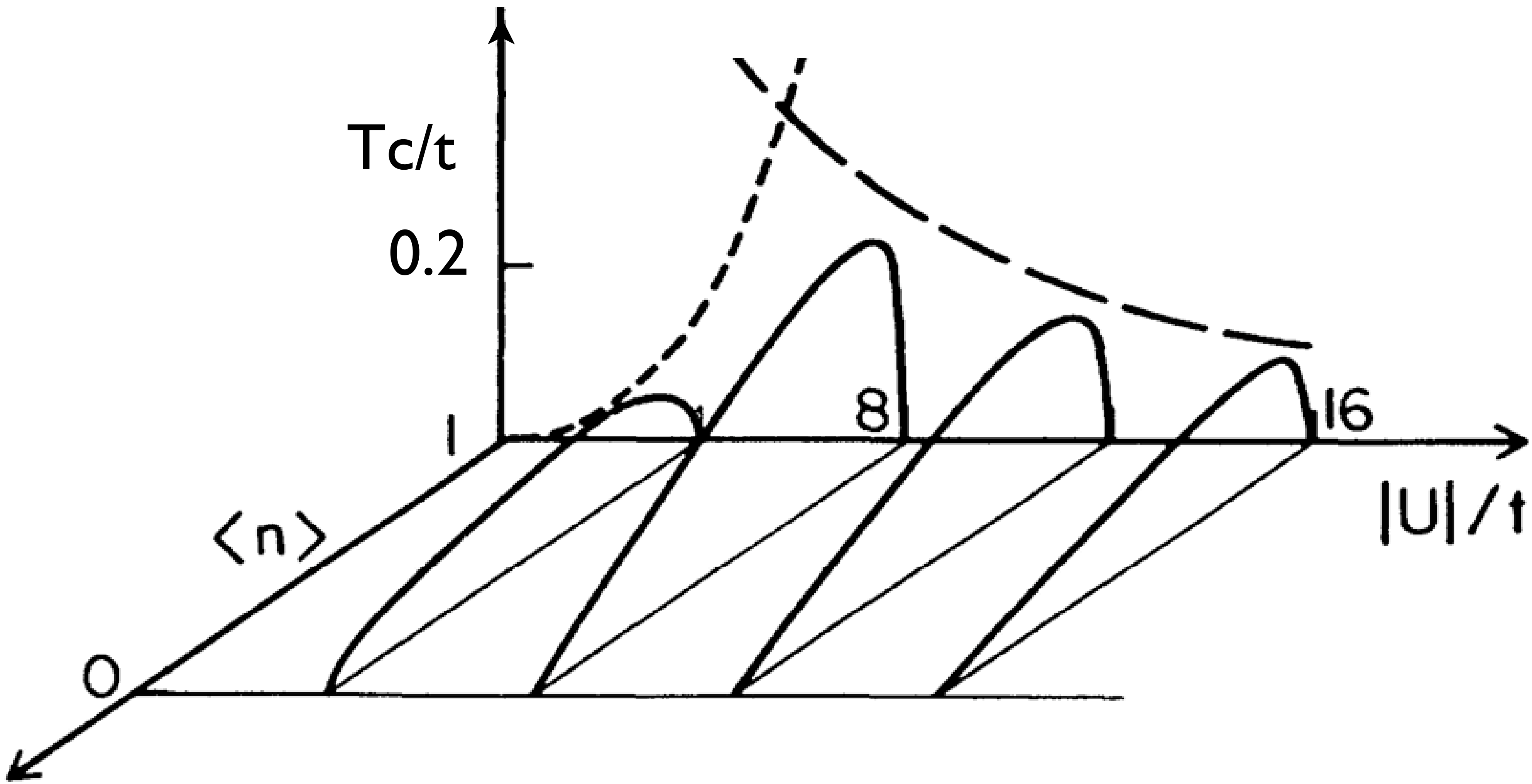
U/t=−4, <n>=0.87
P_s, $S(\pi,\pi)$ 4x4
P_s, $S(\pi,\pi)$ 6x6
P_s, $S(\pi,\pi)$ 8x8
$S(\pi,\pi)$
(b)
0
2
4
6
8
10
β

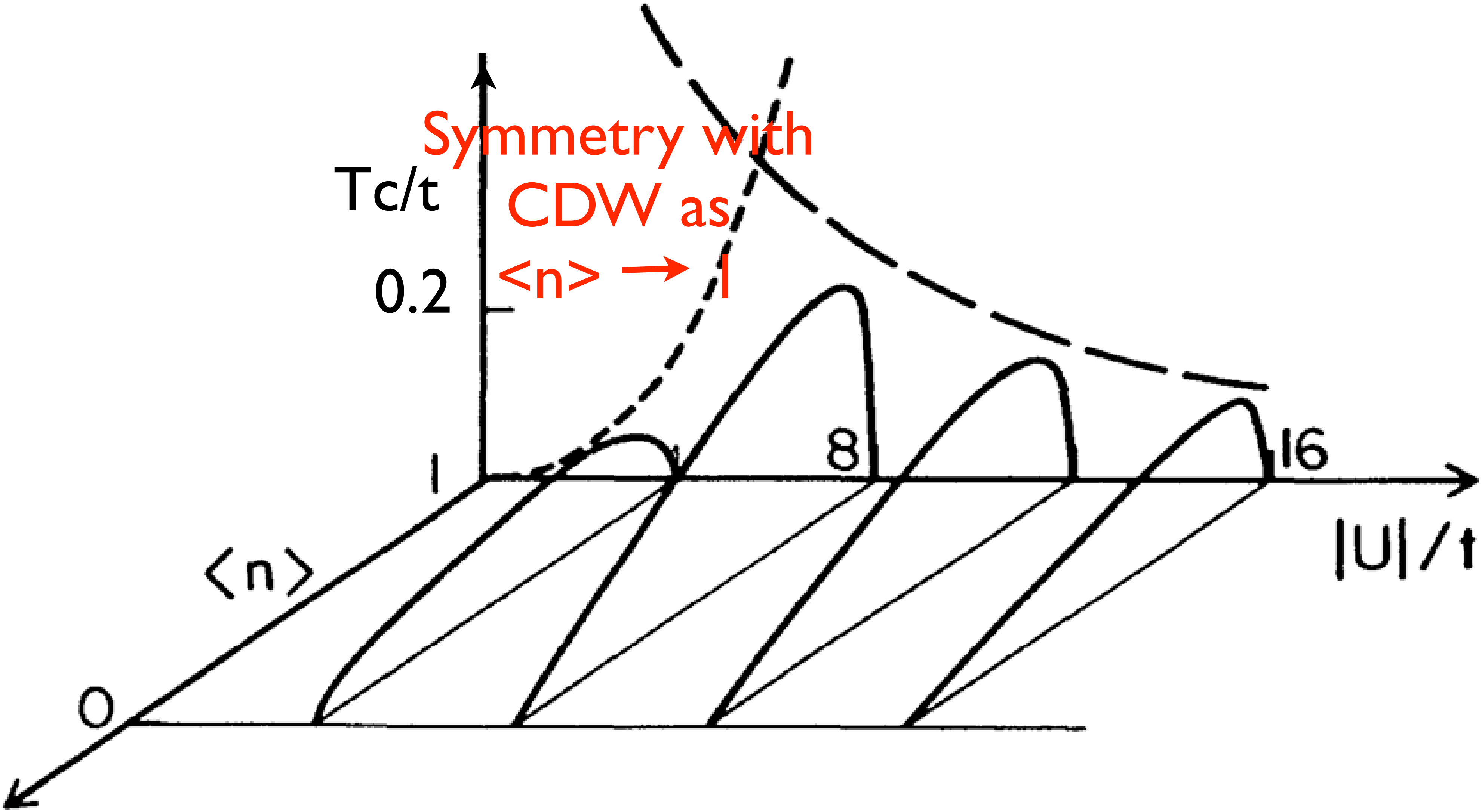
T.Paiva et. al. PRB 69, 184501 (2004)

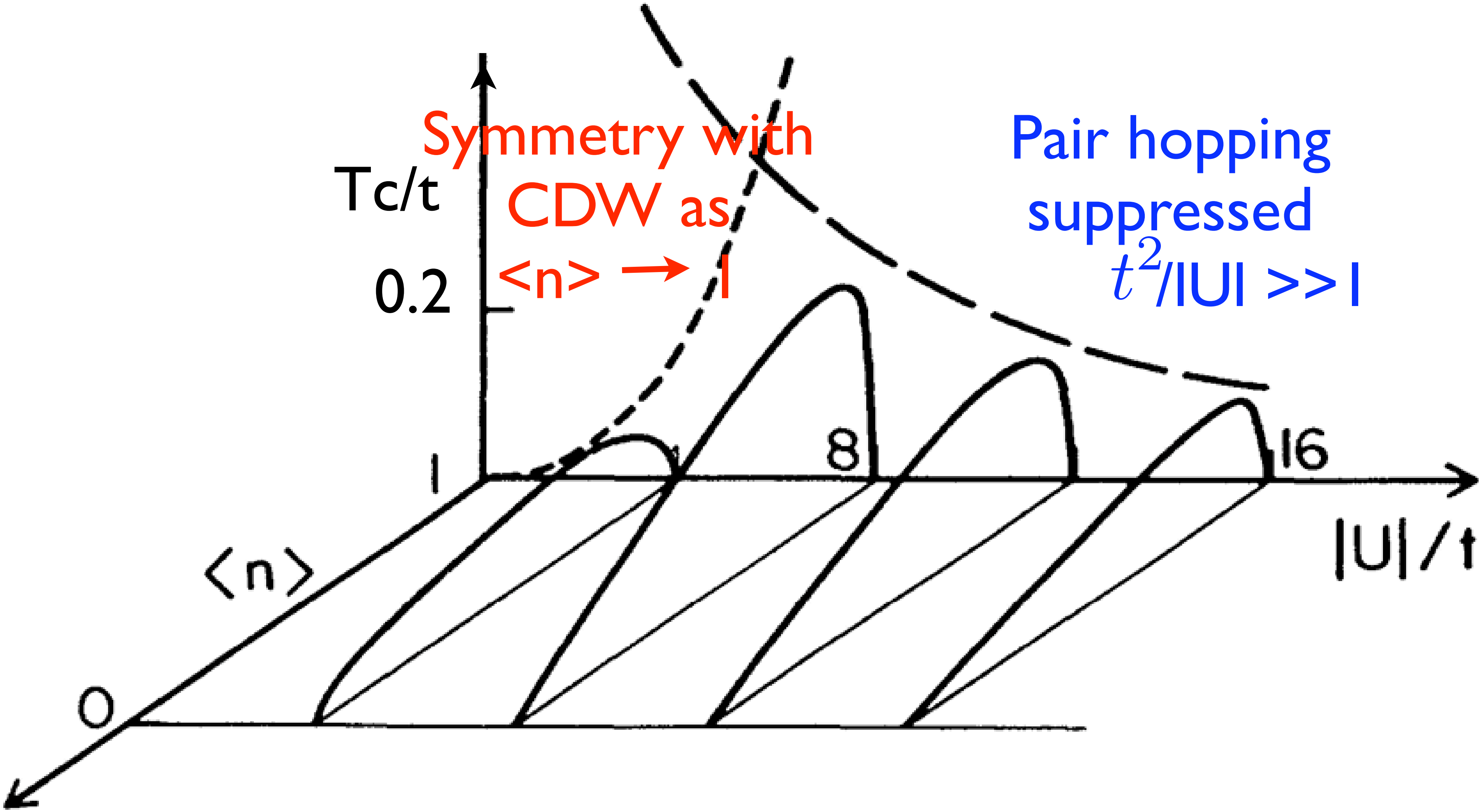



0.2
Tc/t
0.1
<n>=0.6
4
8
12
|U|/t

Schematic Phase Diagram for the negative U Hubbard model




Symmetry with
CDW as
<n> → 1
Tc/t
0.2
1
8
16
|U|/t
<n>
0


Symmetry with
CDW as
<n> → 1
Pair hopping
suppressed
t^2/|U| >>1
Tc/t
0.2
1
8
16
|U|/t
<n>
0

Conclusions for 2D negative U Hubbard

At half-filling SU(2) pairfield and CDW fluctuations suppress Tc to zero. Doping breaks the symmetry and one has a finite temperature superconducting KT transition.

Too large a value of $|U|$ suppresses T_c.

Doped away from half-filling the maximum

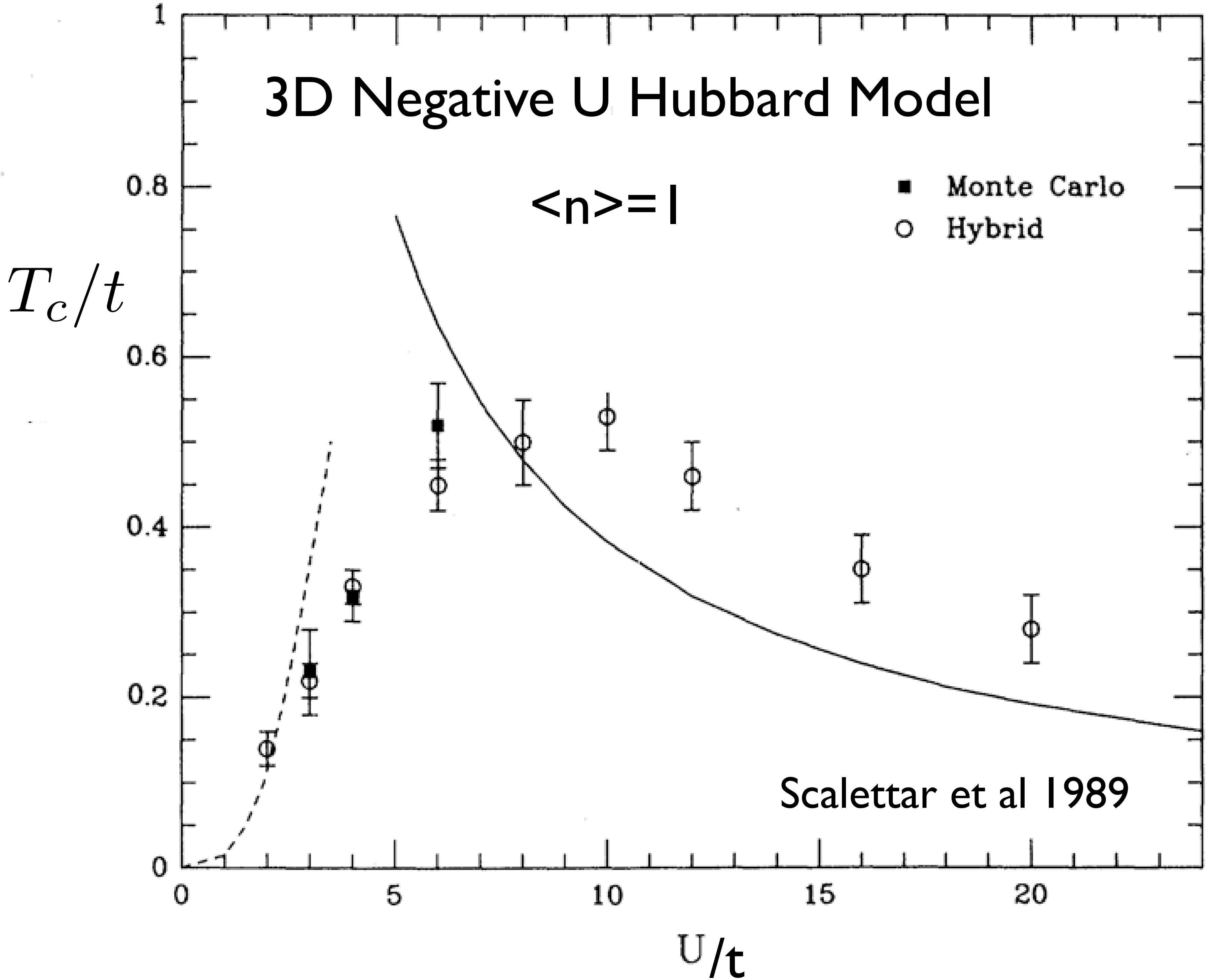
$$T_c \sim 0.2t$$

for the 2-D case is obtained for $|U| \sim 8t$ (the bandwidth)

For T_c=300K one needs

$$t \sim 5T_c = 125\text{meV}$$

$$|U| \sim W = 8t = 1\text{eV}$$


3D Negative U Hubbard Model
<n>=1
Monte Carlo
Hybrid
T_c/t
U/t
Scalettar et al 1989
0
0.2
0.4
0.6
0.8
1
0
5
10
15
20

The Holstein Model

$$H = -t \sum_{<i,j>\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + \omega_0 \sum_i a^\dagger_i a_i$$

$$-\mu \sum_{i,\sigma} n_{i\sigma} + g \sum_{i,\sigma} n_{i\sigma} (a^\dagger_i + a_i)$$

The charge density structure factor

$$S(q) = \frac{1}{N} < \rho_q^\dagger \rho_q > \quad \text{with} \quad \rho_q^\dagger = \sum_{l,\sigma} e^{i\mathbf{q.l}} c_{l\sigma}^\dagger c_{l\sigma}$$

The charge density structure factor

$$S(q) = \frac{1}{N} < \rho_q^\dagger \rho_q > \quad \text{with} \quad \rho_q^\dagger = \sum_{l,\sigma} e^{i\mathbf{q.l}} c_{l\sigma}^\dagger c_{l\sigma}$$

The pairfield susceptibility

$$P_{\mathsf{s}}(T) = \int_0^\beta d\tau < \Delta(\tau)\Delta^\dagger(0) >$$

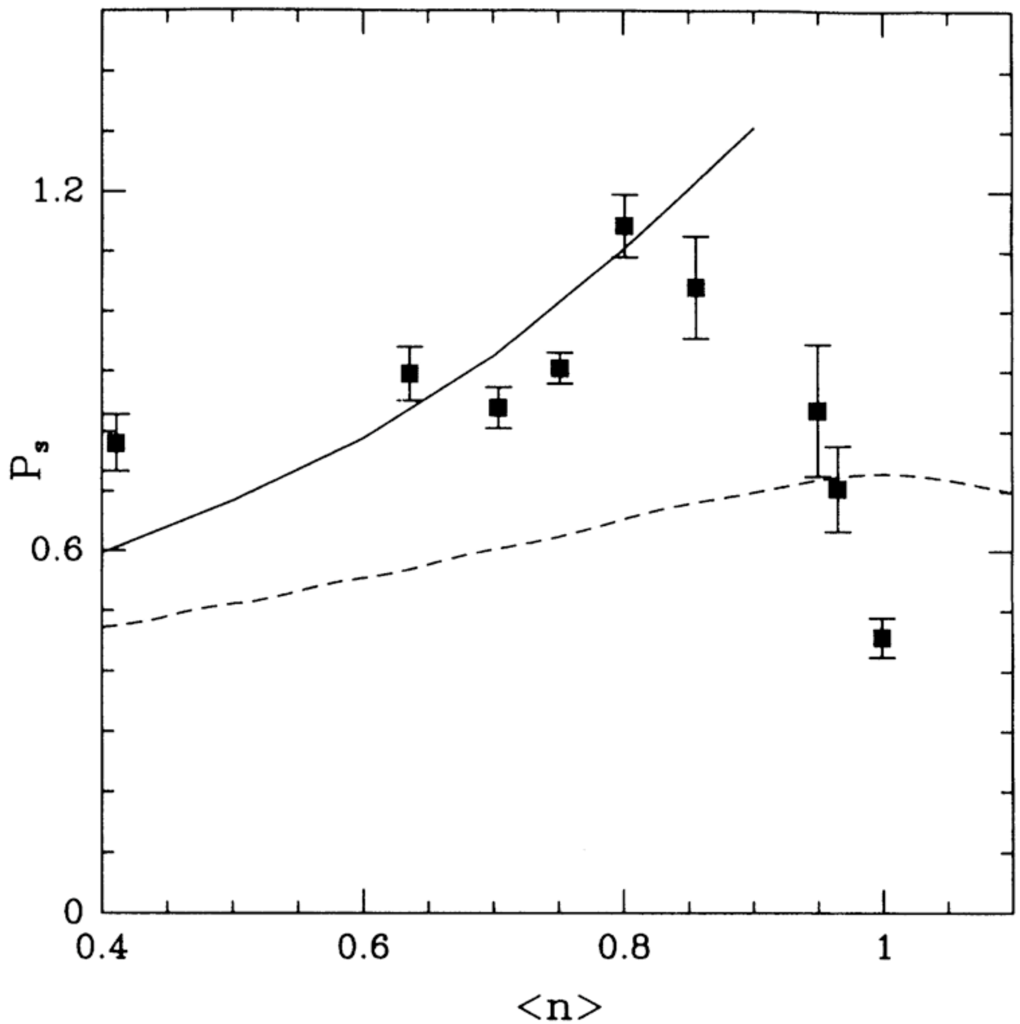
with $$\Delta^\dagger = \frac{1}{\sqrt{N}} \Sigma_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$$

Pair field susceptibility

8x8 lattice $\beta = 12$

$$g = 1 \quad \omega_0 = 1$$

$$\lambda = \frac{2g^2}{D\omega_0} = 0.25$$



Pair field susceptibility

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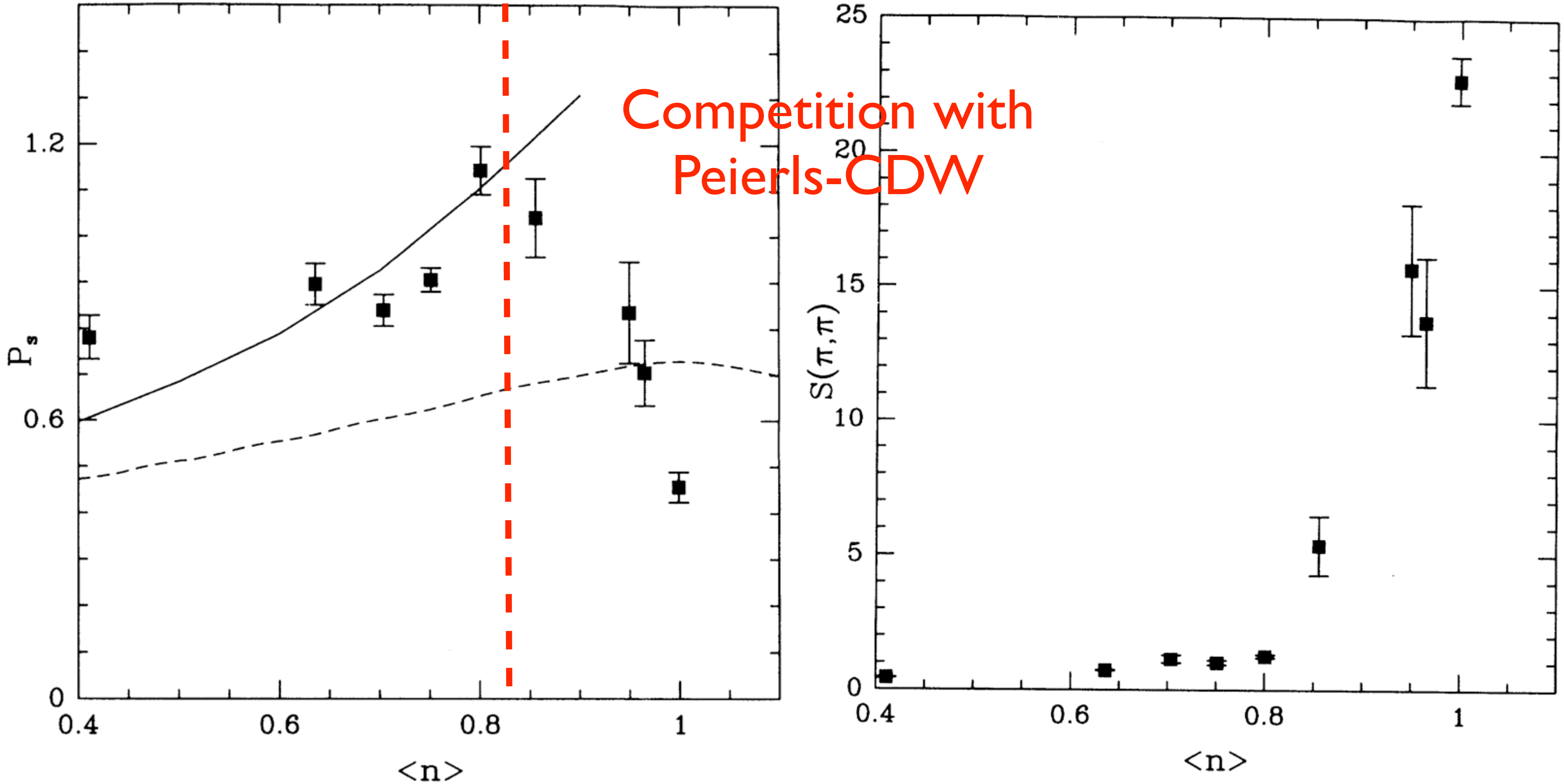
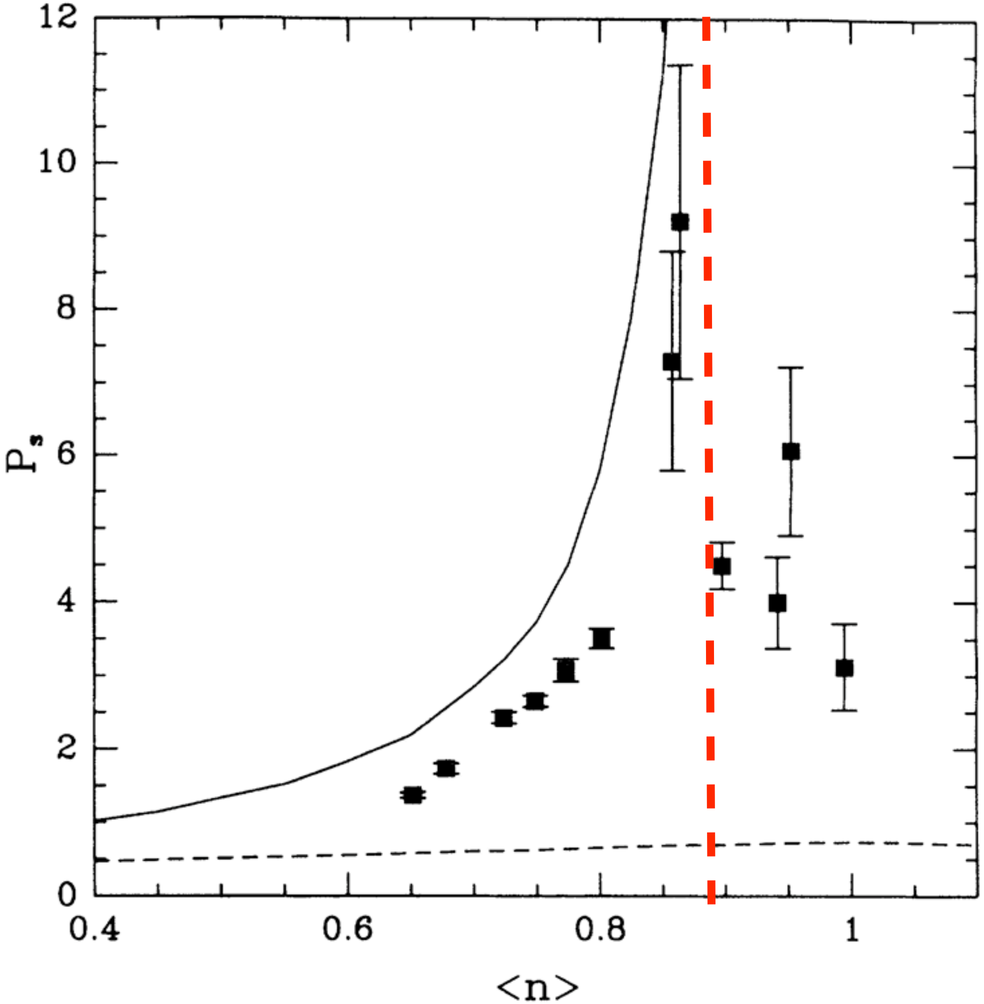
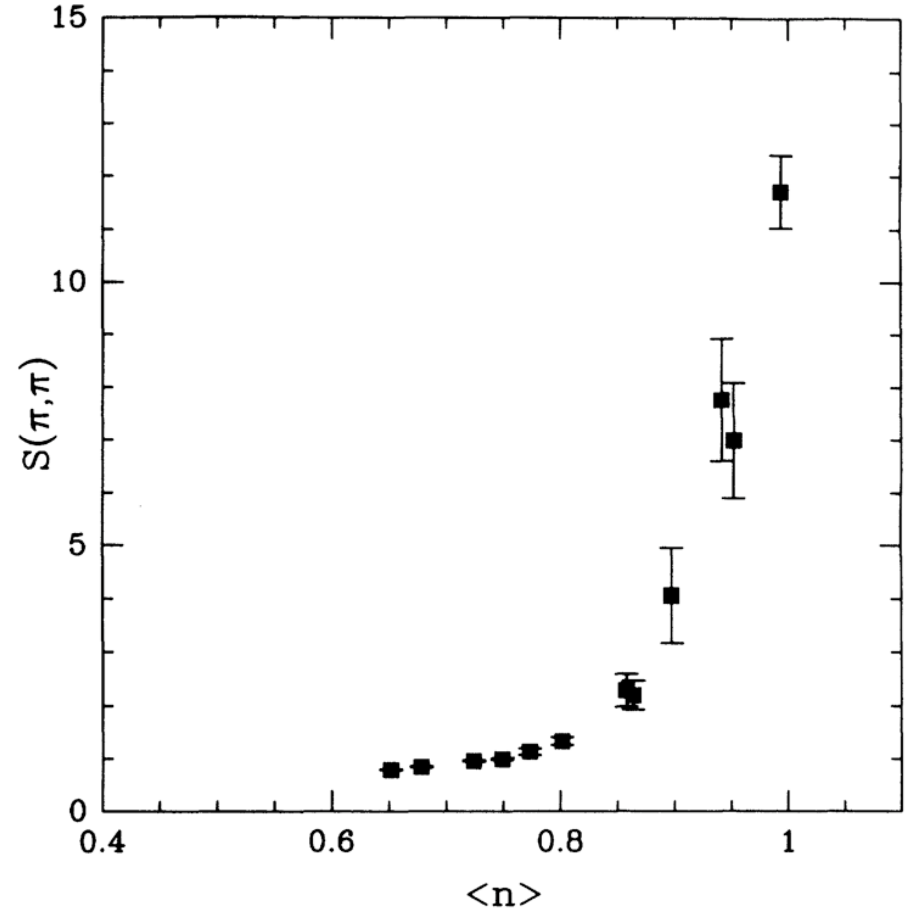
R.M.Noack et al PRL 66 ,778



8x8 lattice $g = 1 \quad \omega_0 = 1$

$\beta = 12$

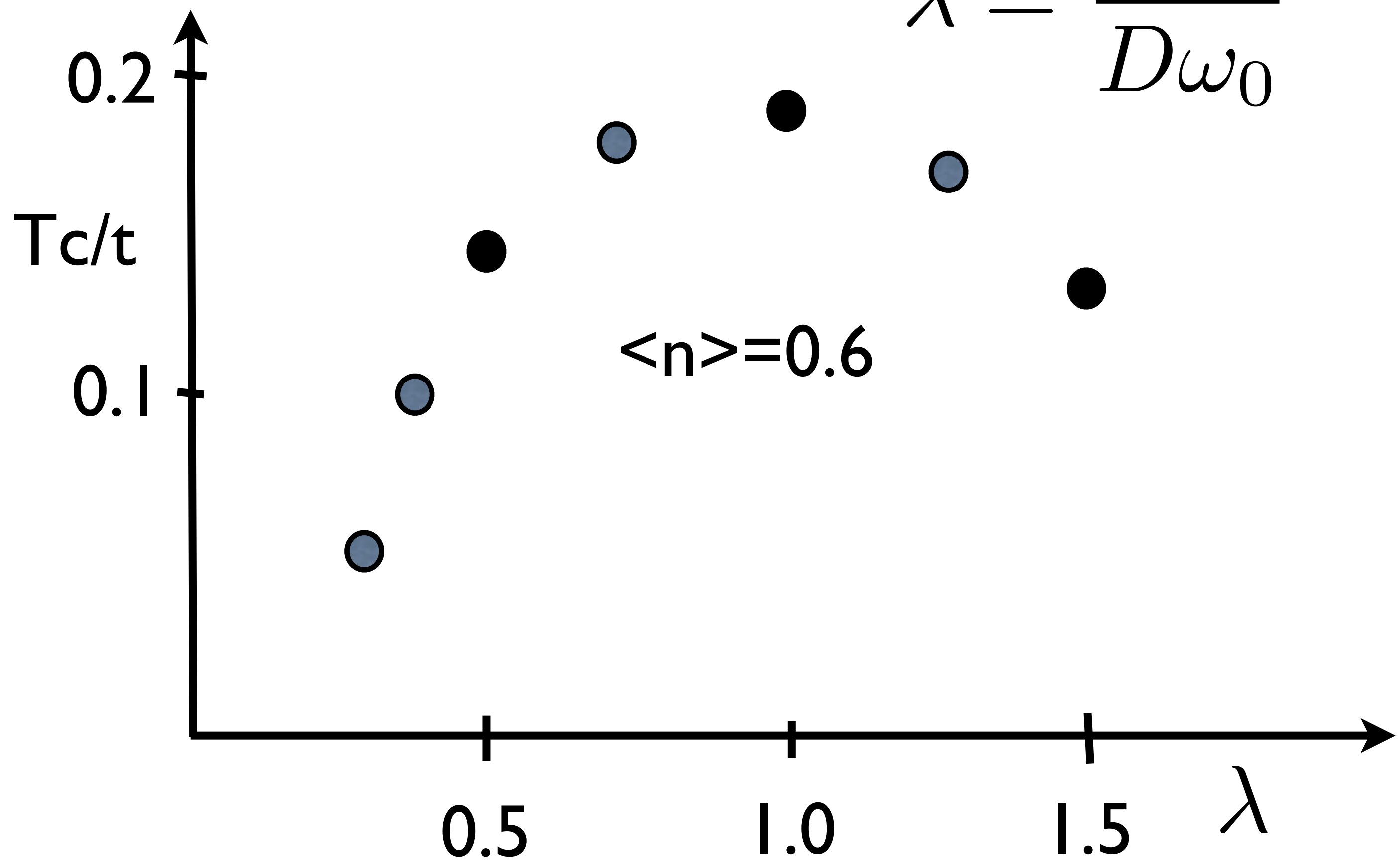




$$\omega_0 = 4 \qquad g = 2 \qquad \lambda = \frac{2g^2}{D\omega_0} = 0.25$$

Schematic

$$\lambda = \frac{2g^2}{D\omega_0}$$



Conclusions for the 2D Holstein Model

The Peierls-CDW phase competes with superconductivity and one needs to dope away from half-filling before one finds a superconducting phase.

Too strong a pairing interaction suppresses Tc.

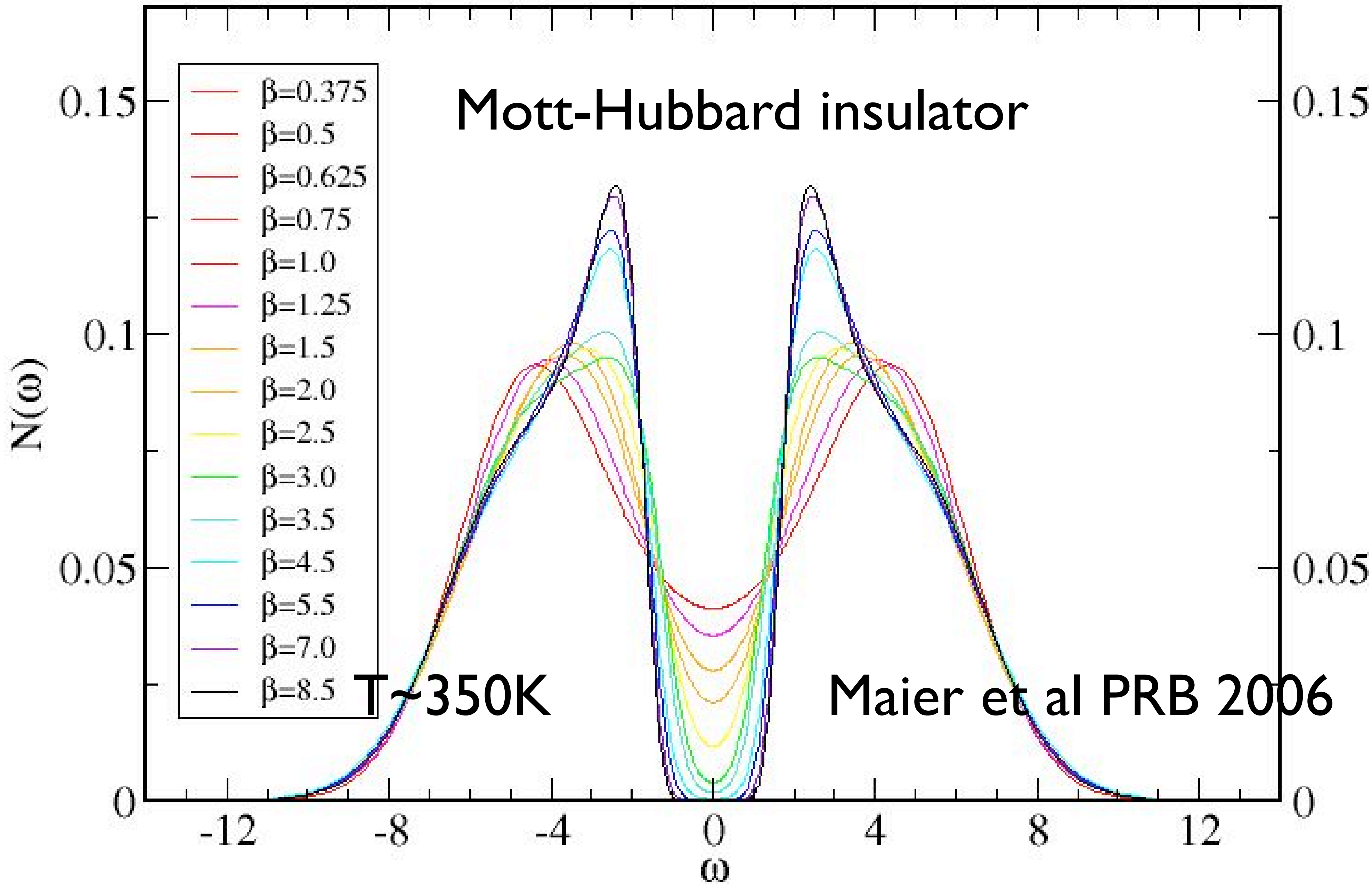
It appears that for the 2D holstein model having ω_0~t and

$$\lambda = \frac{2g^2 N(0)}{\omega_0} \sim \frac{2g^2}{\omega_0 8t} \sim 1$$

gives the maximum Tc . .

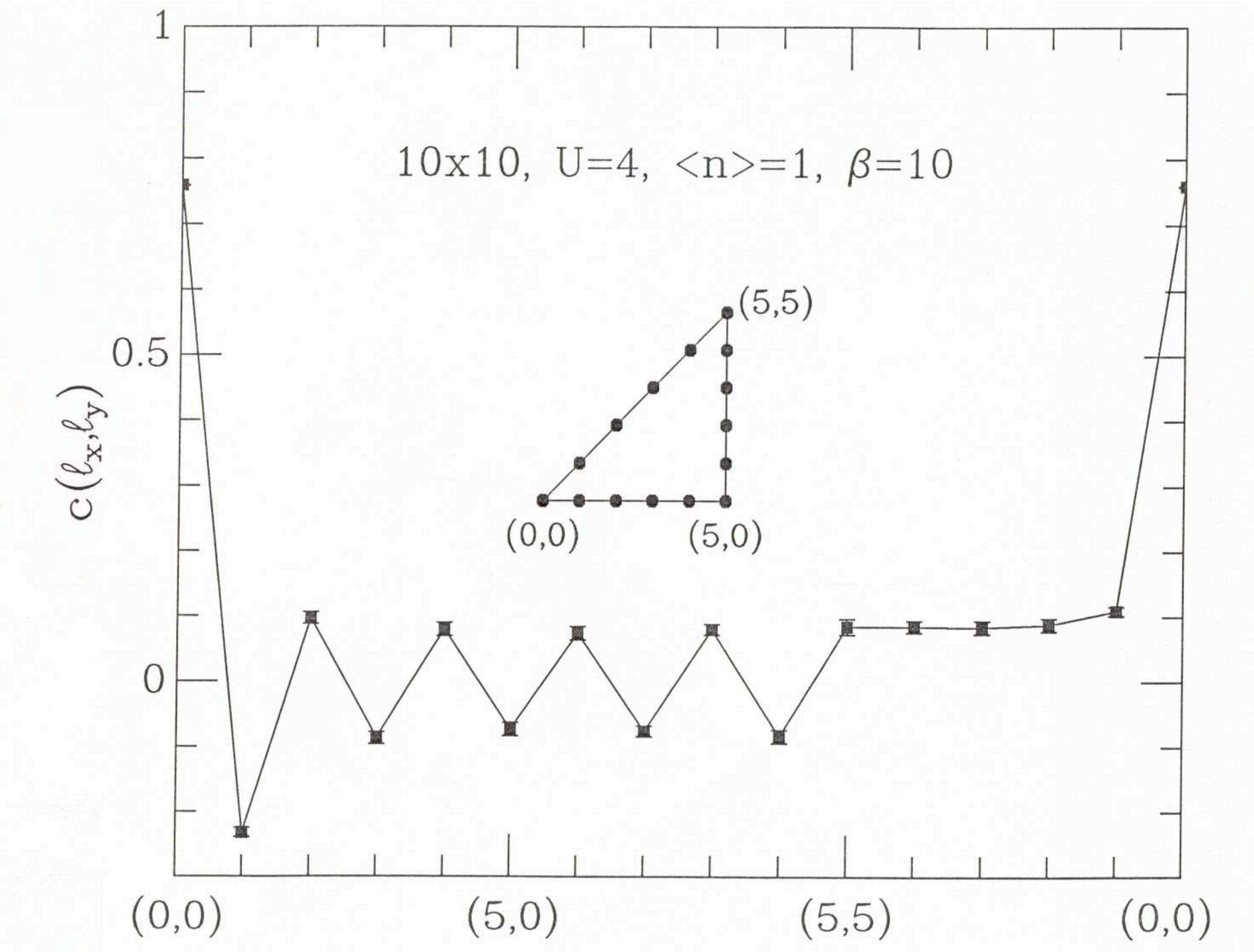
The 2D positive U Hubbard model

Single Particle Density of States
U=8t <n>=1.0



$$C(l_x, l_y) = < m_z(l_x, l_y) m_z(0,0) >$$

$$m_z = n_\uparrow - n_\downarrow$$



Antiferromagnetic Ground State

Hirsch PRB '85

The 2D positive U Hubbard model

At half-filling the ground state of the positive U Hubbard model is an insulating anti-ferromagnet.

The 2D positive U Hubbard model

At half-filling the ground state of the positive U Hubbard model is an insulating anti-ferromagnet.

The doped system exhibits d-wave pairing correlations and stripes.

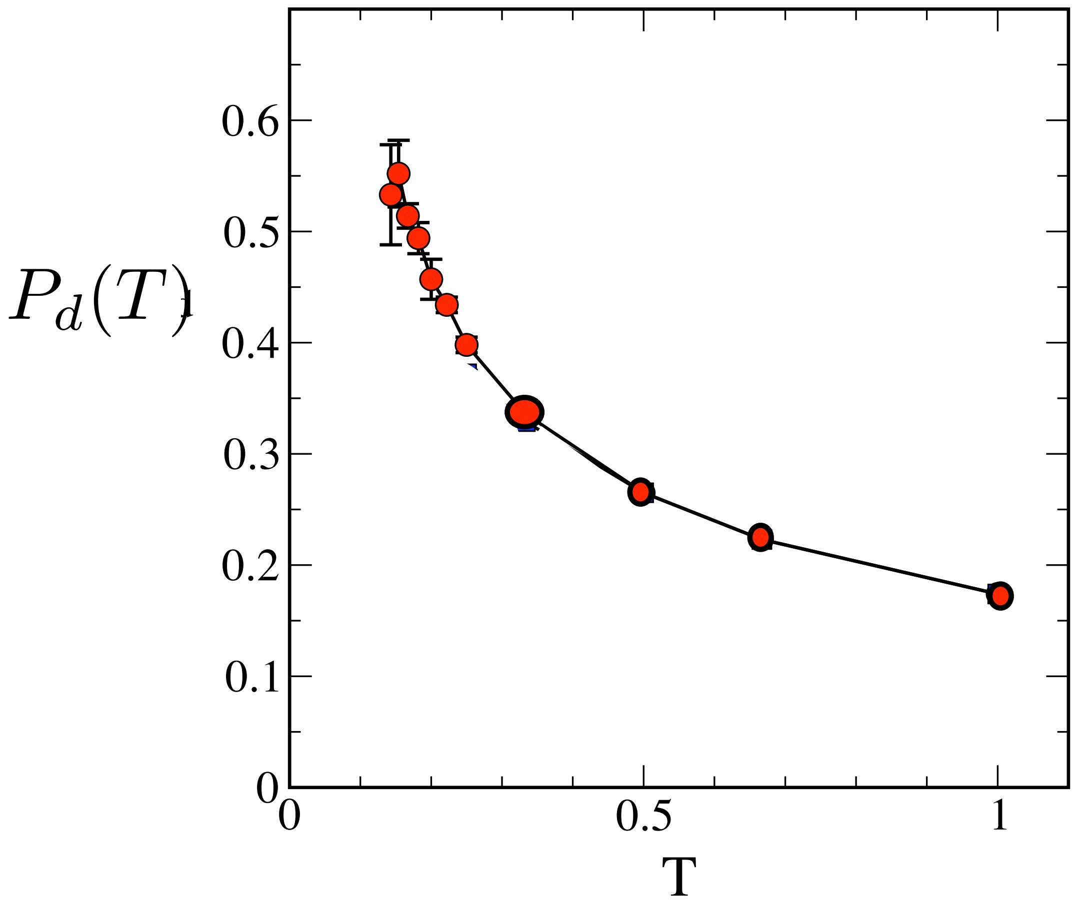
The D-wave pairfield susceptibility

$$P_d = \int_0^\beta d\tau \, \langle \Delta_d(\tau) \, \Delta_d^\dagger(0) \rangle$$

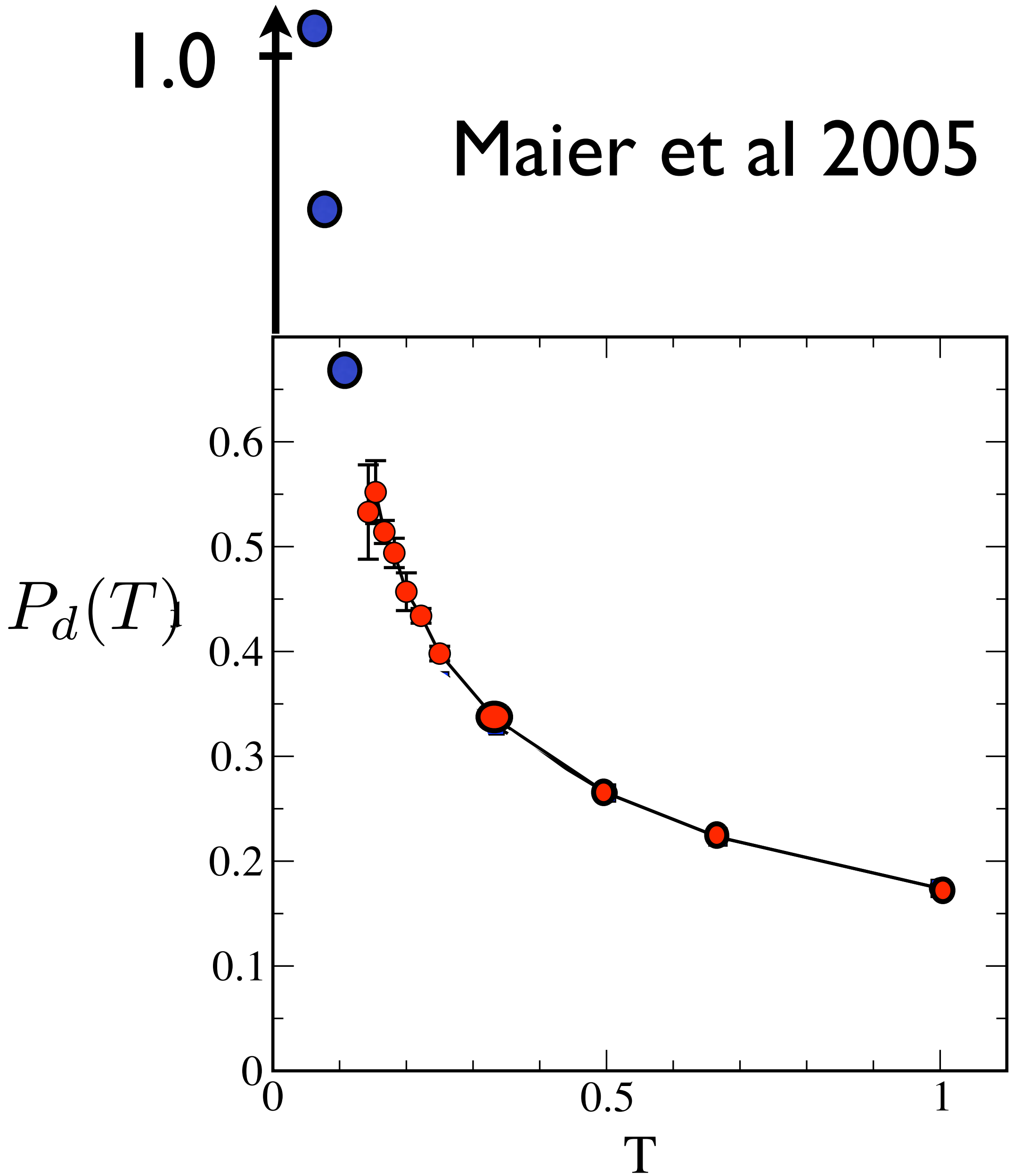
$$\Delta_d^\dagger = \frac{1}{2\sqrt{N}} \sum_{\ell,\delta} (-1)^\delta c_{\ell\uparrow}^\dagger c_{\ell+\delta\downarrow}^\dagger$$

$$P_d = \int_0^\beta d\tau \, \langle \Delta_d(\tau) \, \Delta_d^\dagger(0) \rangle$$

$$\Delta_d^\dagger = \frac{1}{2\sqrt{N}} \sum_{\ell.\delta} (-1)^\delta c_{\ell\uparrow}^\dagger c_{\ell+\delta\downarrow}^\dagger$$

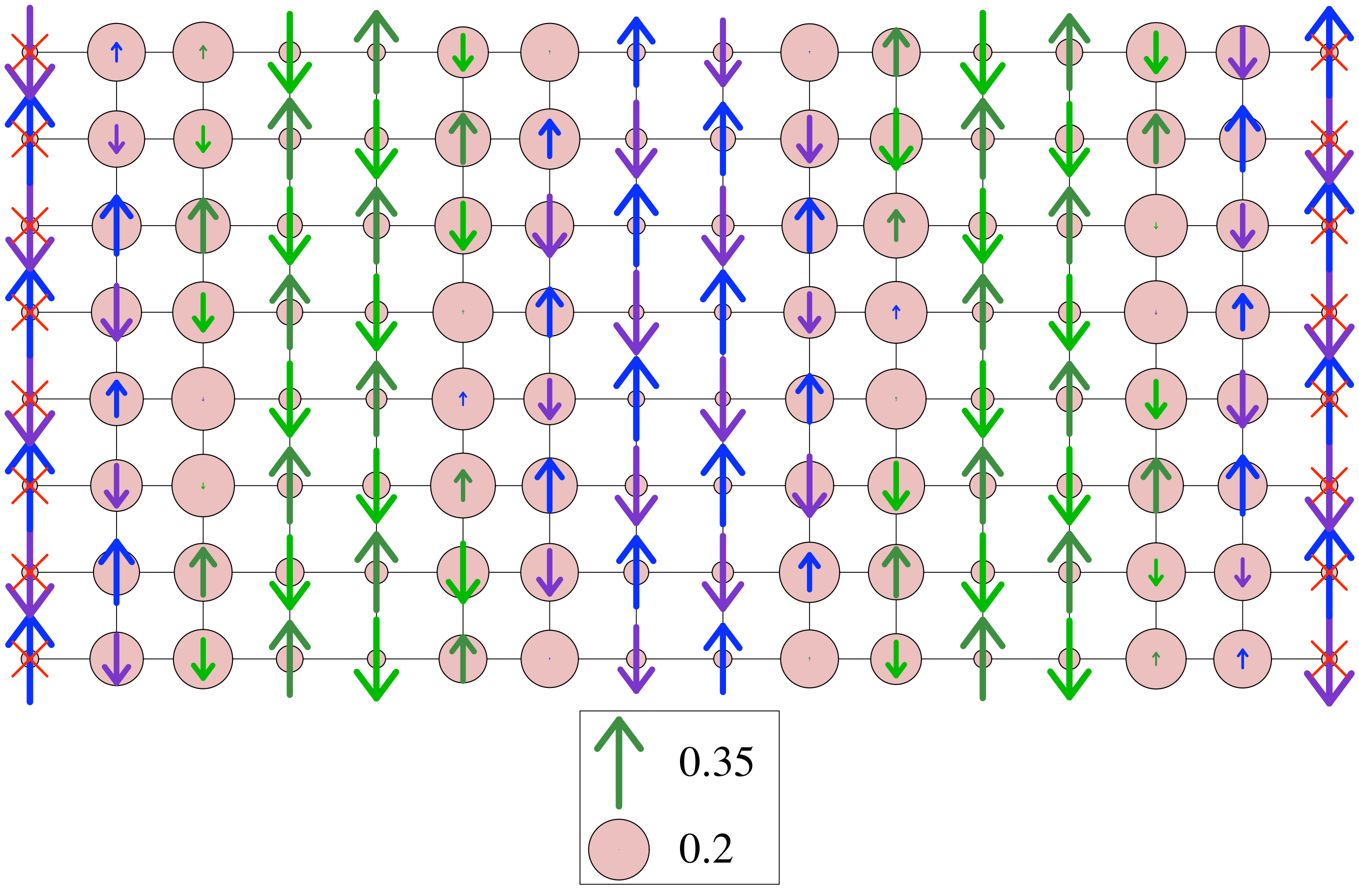


Loh et al, PRB '90



Loh et al, PRB '90

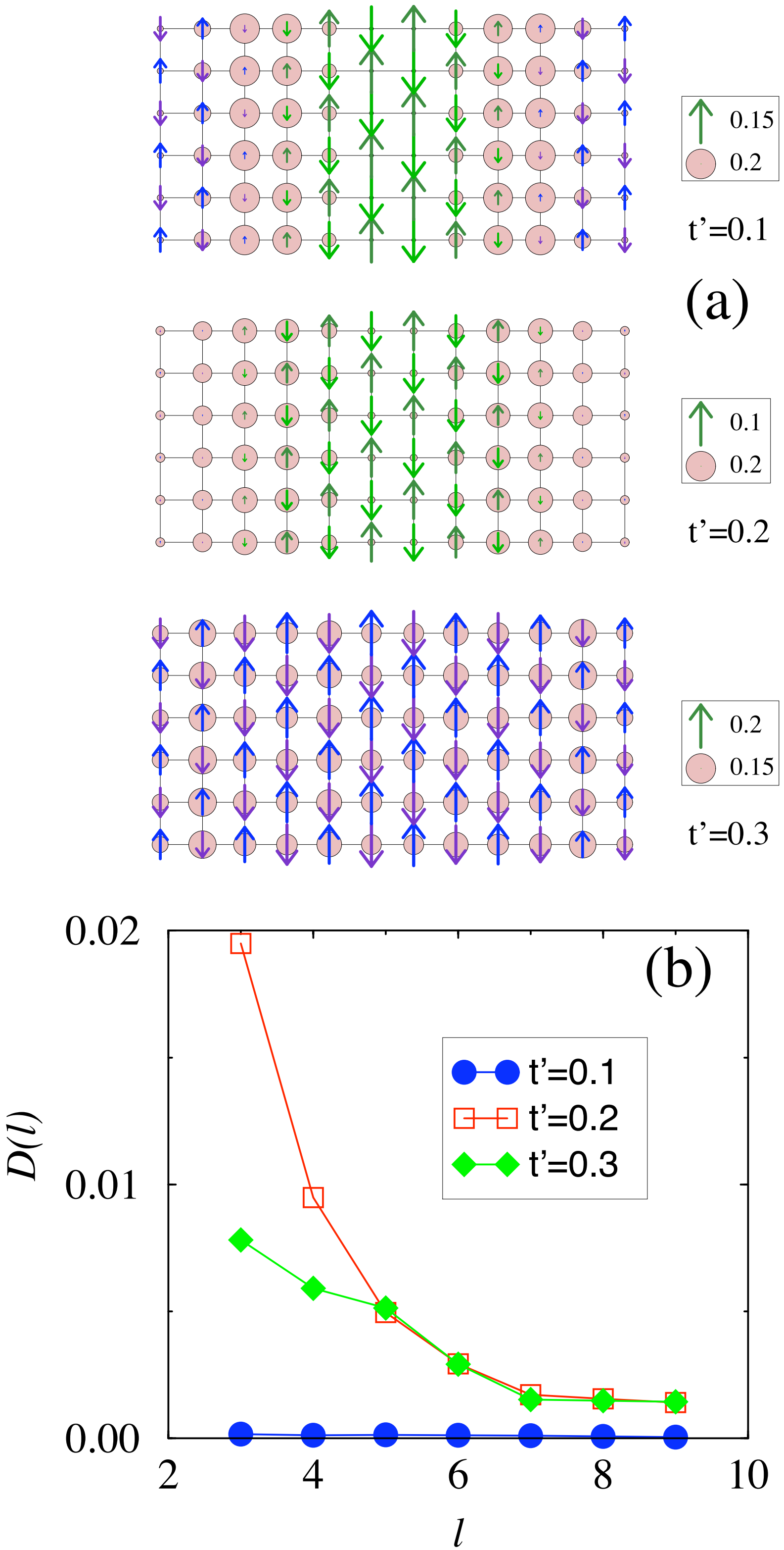
Stripes



16 x 8 system, Vertical PBC's

x=1/8   16 holes

White and Scalapino



0.15
0.2
t'=0.1
(a)
0.1
0.2
t'=0.2
0.2
0.15
t'=0.3
(b)
D(l)
l
t'=0.1
t'=0.2
t'=0.3
0.02
0.01
0.00
2
4
6
8
10

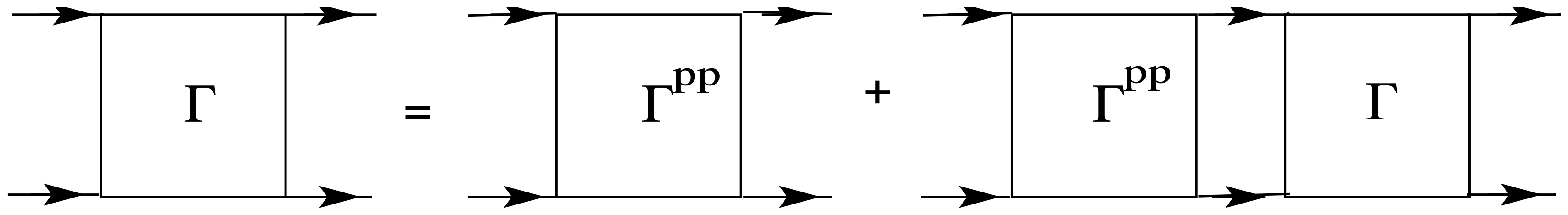
The 2D positive U Hubbard model

At half-filling the ground state of the positive U Hubbard model is an insulating anti-ferromagnet.

The doped system exhibits d-wave pairing correlations and stripes.

The $x=1/8$ striped state competes with the d-wave correlations.

The pairing interaction is given by the irreducible particle-particle vertex Γ^{pp}

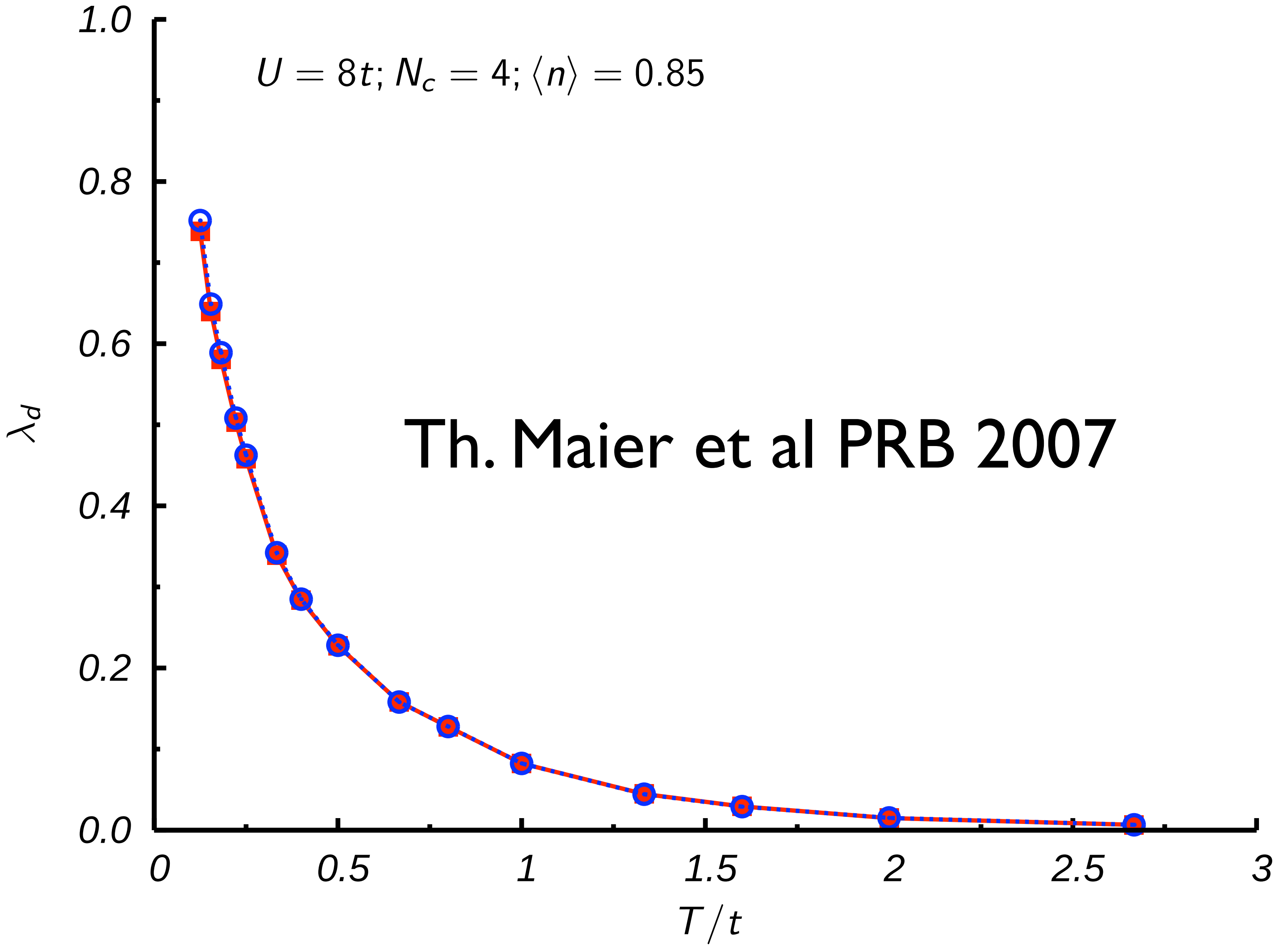


The Bethe-Salpeter equation for the particle-particle channel with a center of mass momentum Q=0 is the generalization of the BCS equation

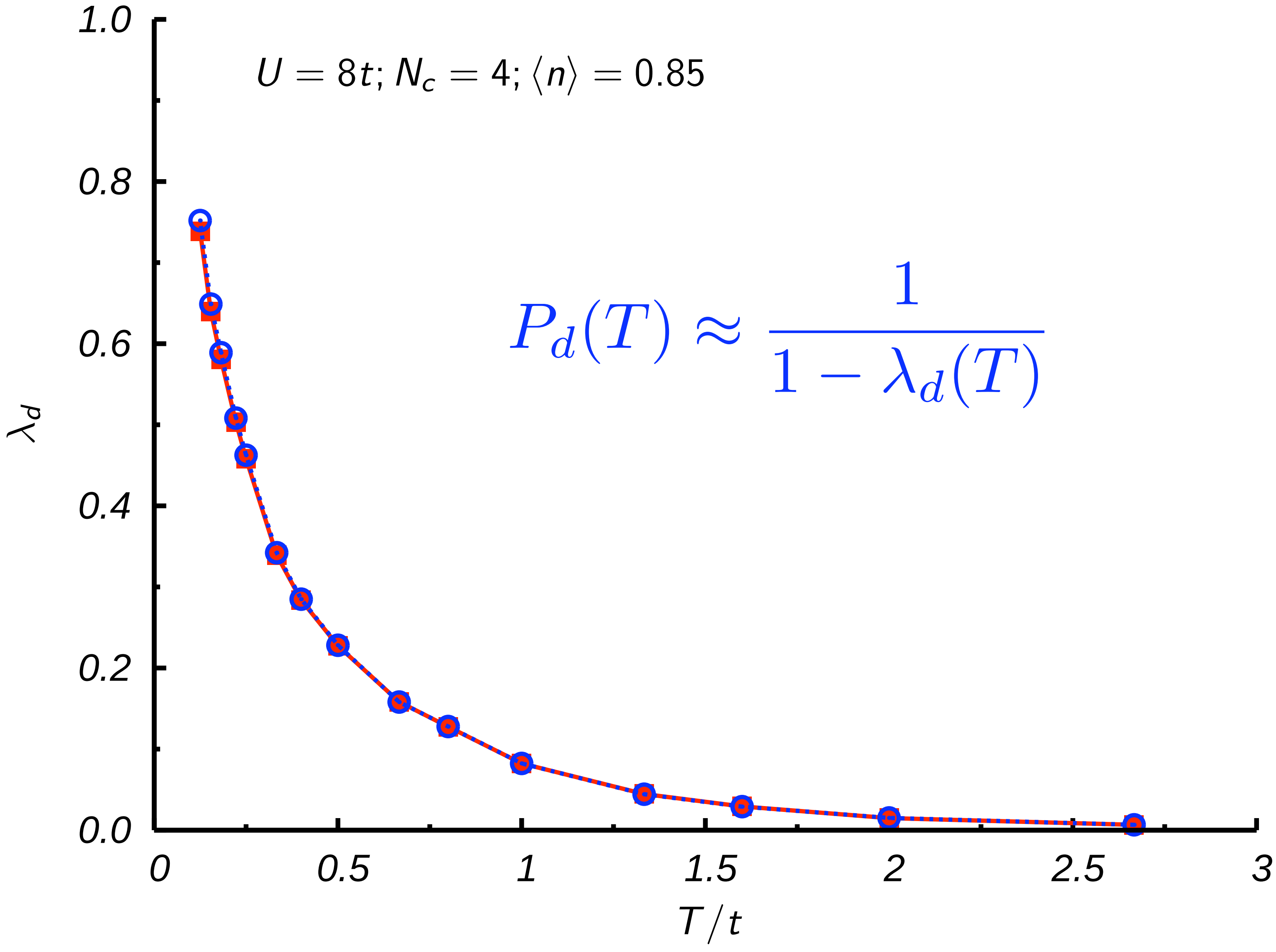
$$-(T/N)\sum_{p'}\Gamma^{pp}(p;p')G(p')G(-p')\phi_\alpha(p') = \lambda_\alpha\phi_\alpha(p)$$

$p = (\mathbf{p}, i\omega_n)$ when $\lambda_d = 1, T = T_c$

.

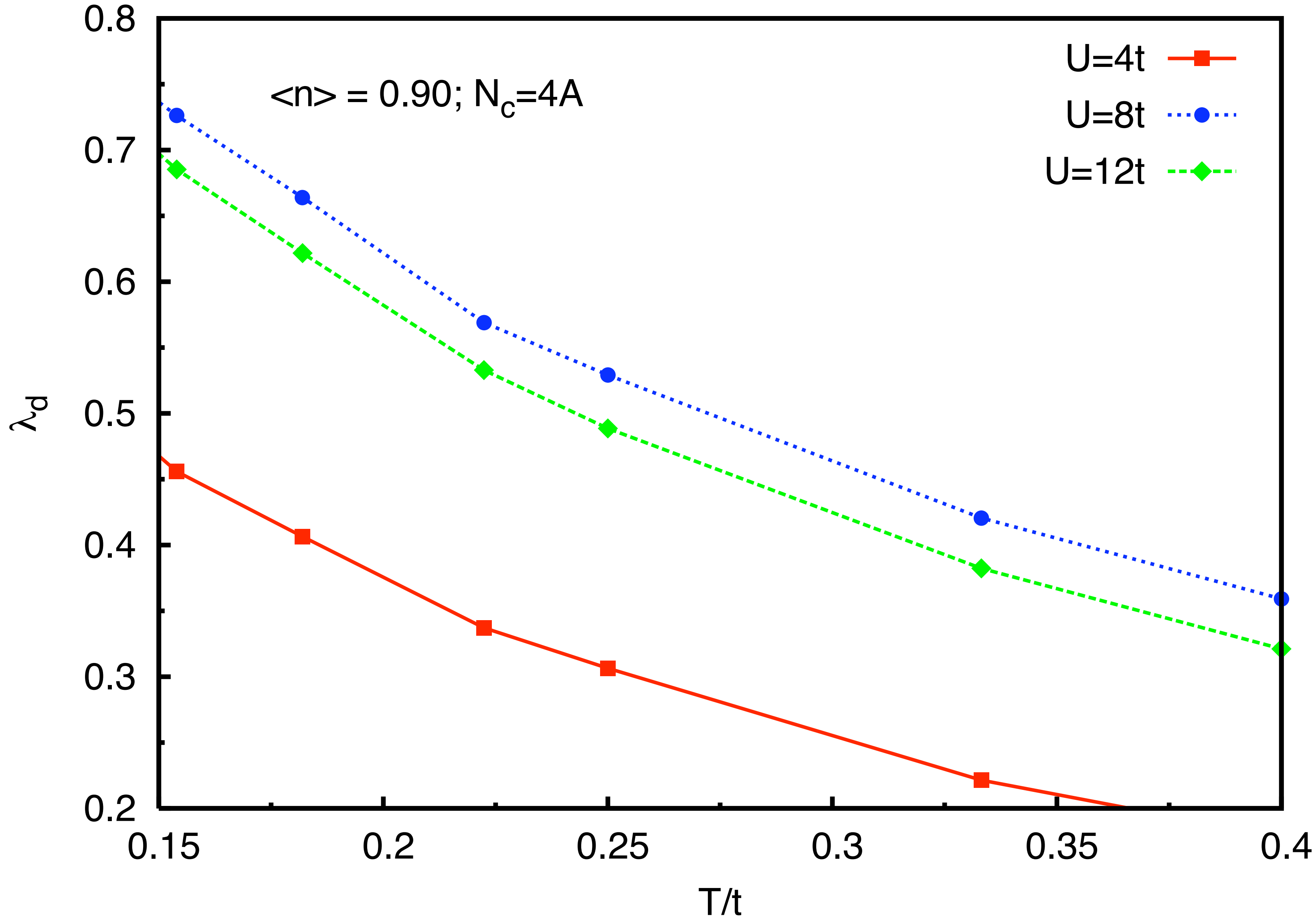


$U = 8t; N_c = 4; \langle n \rangle = 0.85$
Th. Maier et al PRB 2007
λ_d
1.0
0.8
0.6
0.4
0.2
0.0
0
0.5
1
1.5
2
2.5
3
T/t



$U = 8t;\ N_c = 4;\ \langle n \rangle = 0.85$
$P_d(T) \approx \frac{1}{1-\lambda_d(T)}$
λ_d
T/t
1.0
0.8
0.6
0.4
0.2
0.0
0
0.5
1
1.5
2
2.5
3

The d-wave eigenvalue versus T for different values of U



The 2D positive U Hubbard model

At half-filling the ground state of the positive U Hubbard model is an insulating anti-ferromagnet.

The doped system exhibits d-wave pairing correlations and stripes.

The x=1/8 striped state competes with the d-wave correlations.

The optimum U is of order the bandwidth 8t.

For U~8t and <n>~0.85

Tc~0.05t

For Tc=300K one needs t~.50 or
8t~U~4 eV

Retardation

Structure and microstructure

Structure and microstructure

Increasing the strength of the interaction

Negative U

Phys. Rev. B 32, 5639 - 5643 (1985)

Double-valence-fluctuating molecules and superconductivity

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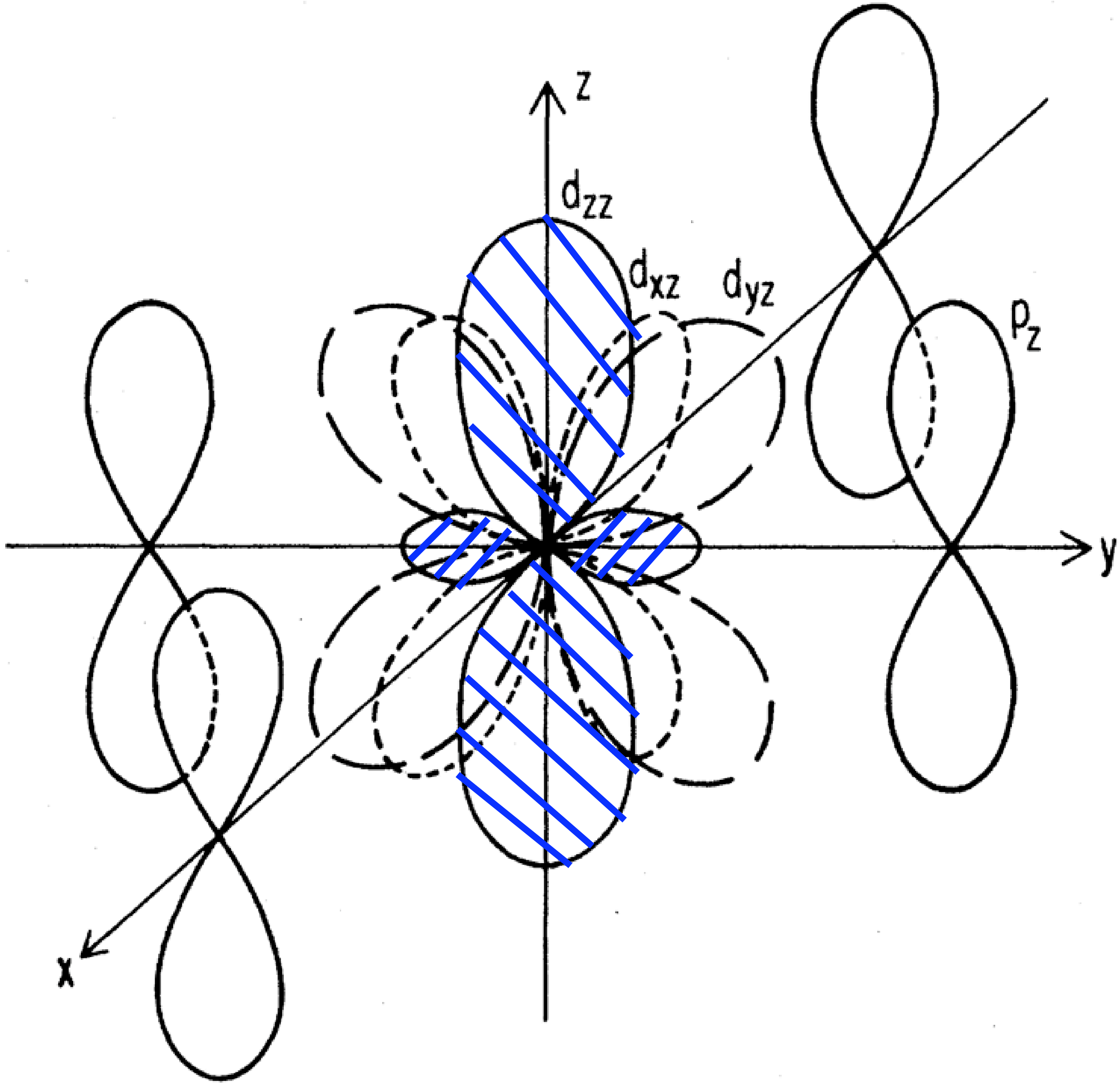
Department of Physics, University of California, Santa Barbara, California 93106

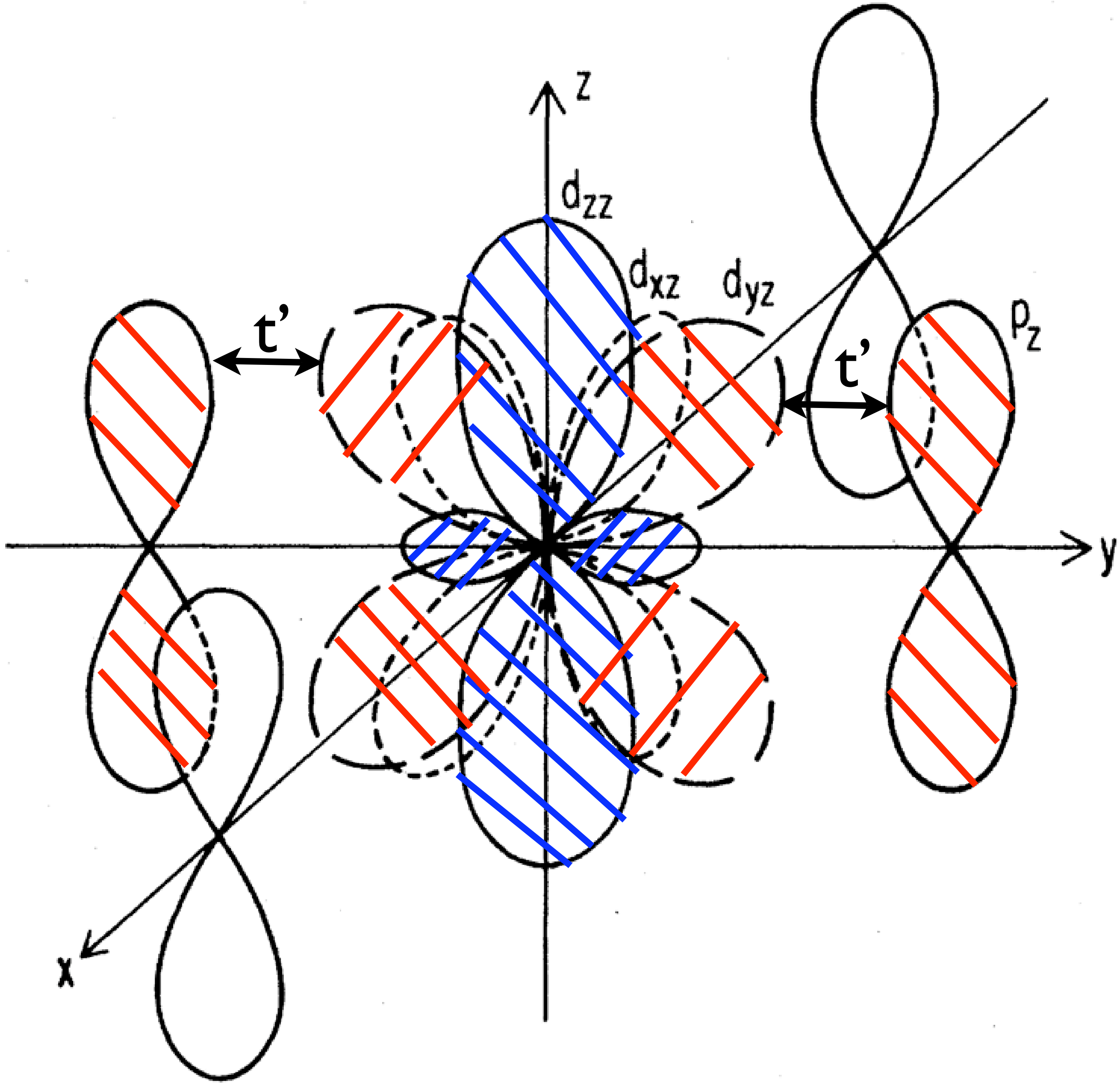
Received 4 June 1985

We discuss the possibility of ‘‘double-valence-fluctuating’’ molecules, having two ground-state configurations differing by two electrons. We propose a possible realization of such a molecule, and experimental ways to look for it. We argue that a weakly coupled array of such molecules should give rise to a strong-coupling Shafroth-Blatt-Butler superconductor, with a high transition temperature.

Double -valence -fluctuating molecule



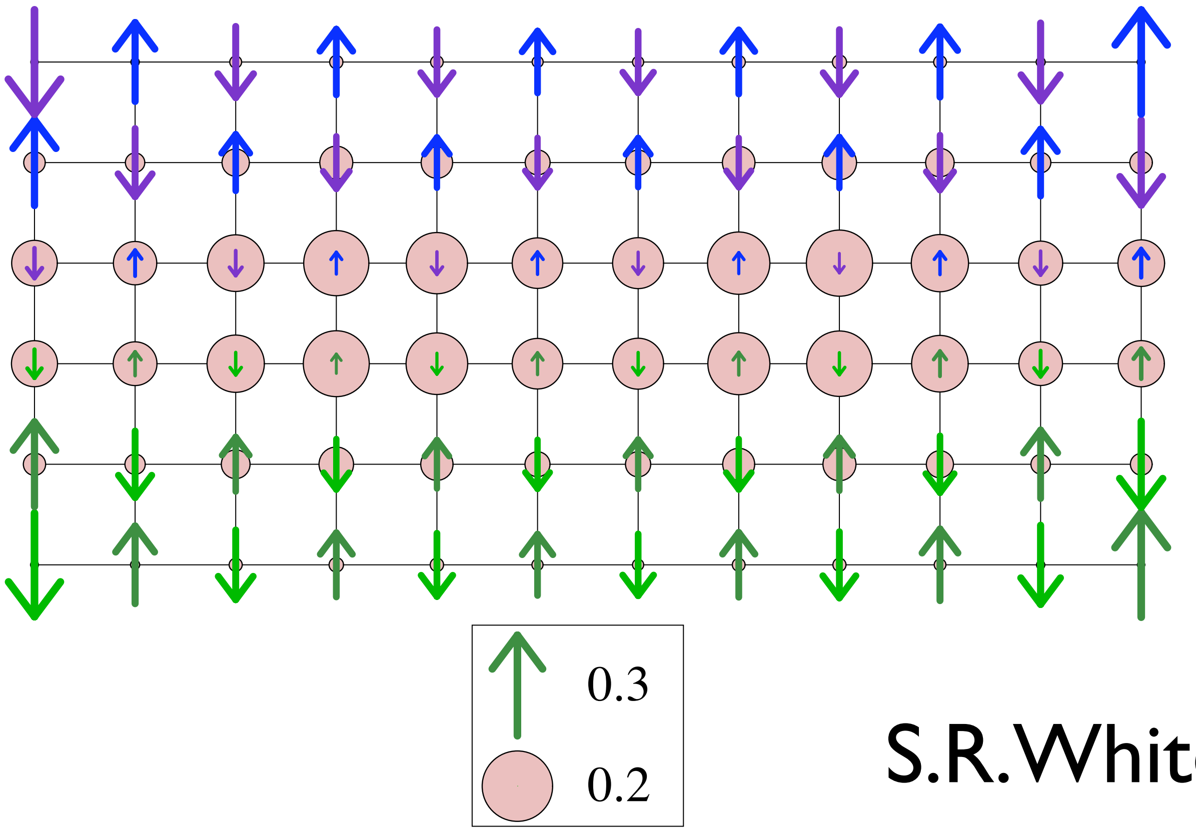
Negative U=E(2)+E(0)-2E(1)



Microstructure

The role of stripes (Kivelson)

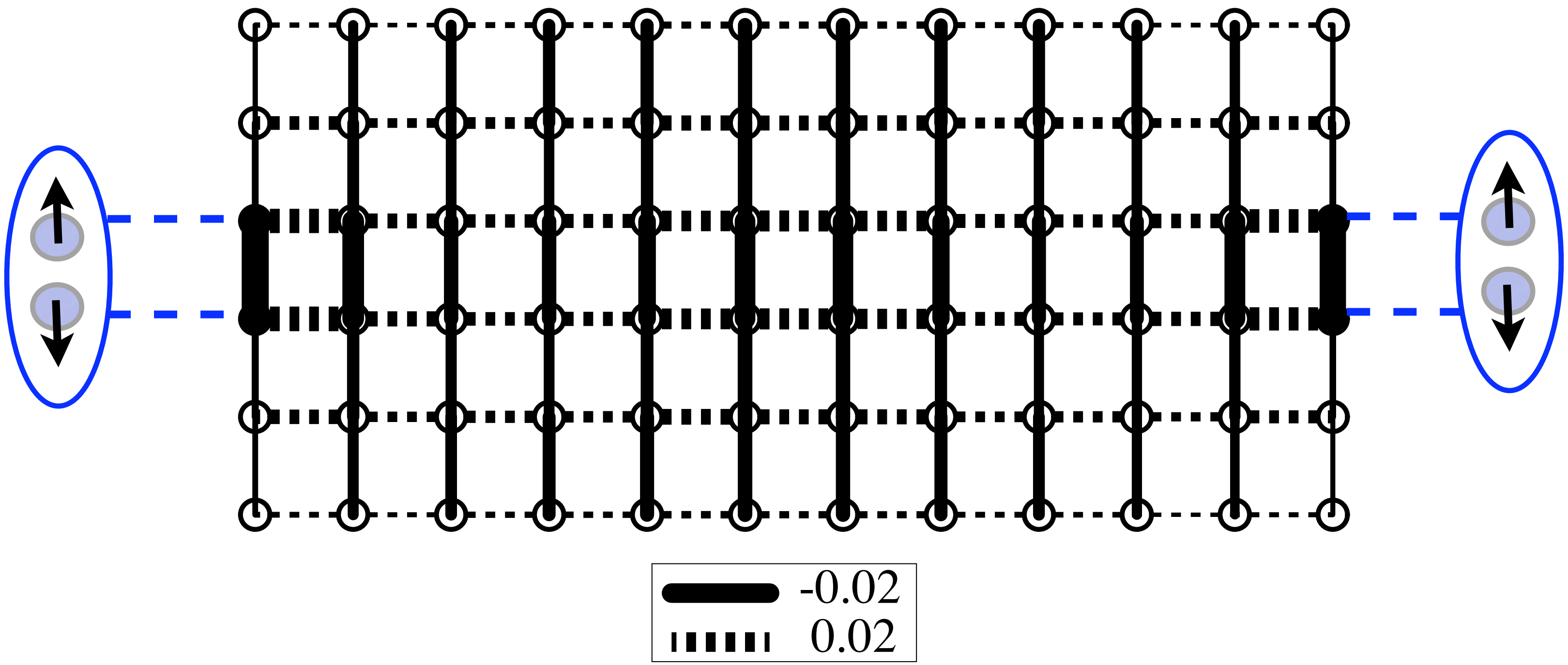
Stripe spin and charge density



S.R.White

12 x 6 system

J/t = 0.5, mu = 1.25, doping = 0.0871



12 x 6 system

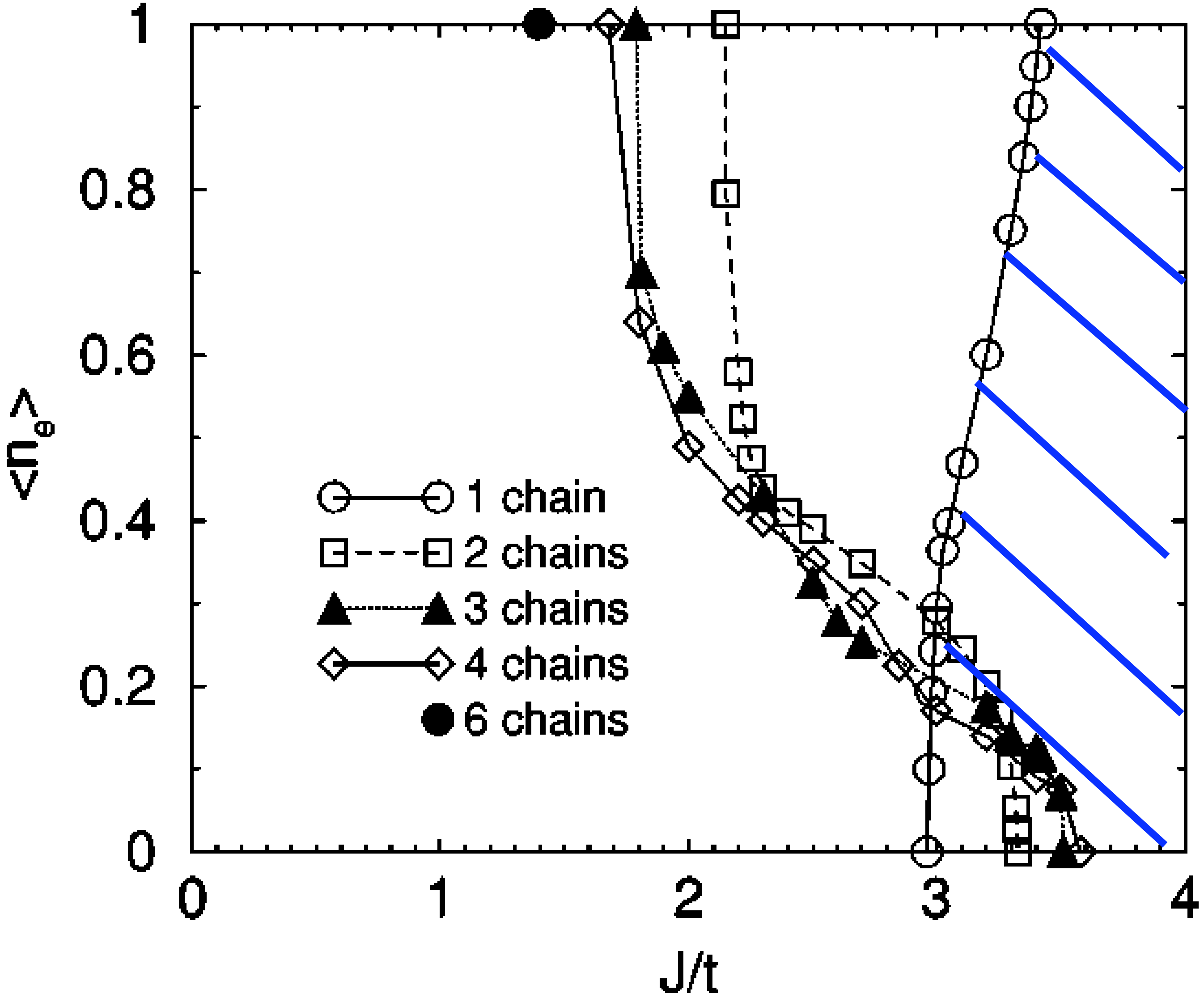
J/t = 0.5, mu = 1.25, doping = 0.0871

Pair-field

Structure

Suppressing competing phases

Phase separation for the 2-leg ladder

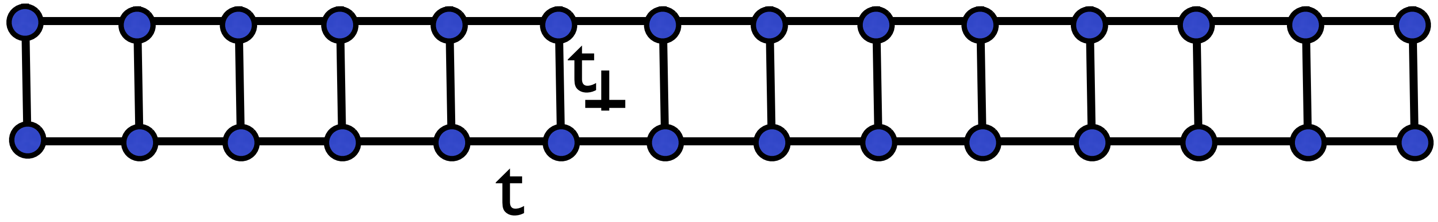


With a weakly coupled 2-leg ladder one can have larger values of J/t with out phase separation. This favors pairing on the ladder.

Structure

Fine tuning

2-leg Hubbard ladder

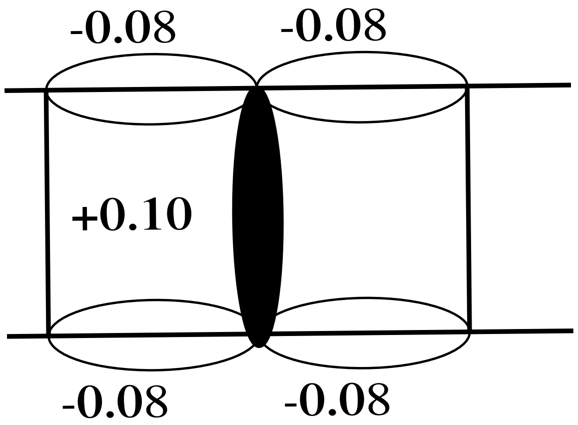


$$H = -t \sum_{i,\lambda\sigma} \left(c^\dagger_{i,\lambda\sigma} c_{i+1,\lambda\sigma} + c^\dagger_{i+1,\lambda\sigma} c_{i,\lambda\sigma} \right)$$

$$- t_\perp \sum_{i,\sigma} \left(c^\dagger_{i,1\sigma} c_{i,2\sigma} + c^\dagger_{i,2\sigma} c_{i,1\sigma} \right) + U \sum_{i,\lambda} n_{i,\lambda\uparrow} n_{i,\lambda\downarrow} \,.$$

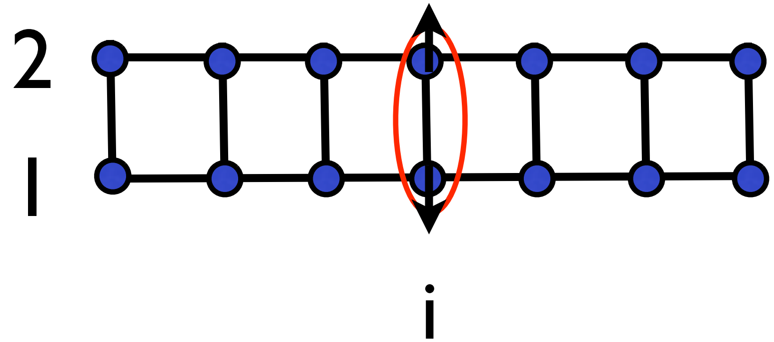
d-wave-like pairfield

$$\left\langle N_2 \left| \left(c^\dagger_{\mathbf{r}\uparrow} c^\dagger_{\mathbf{r}'\downarrow} - c^\dagger_{\mathbf{r}\downarrow} c^\dagger_{\mathbf{r}'\uparrow} \right) \right| N_1 \right\rangle$$



T.M.Rice et al, Europhys. Lett. 1993

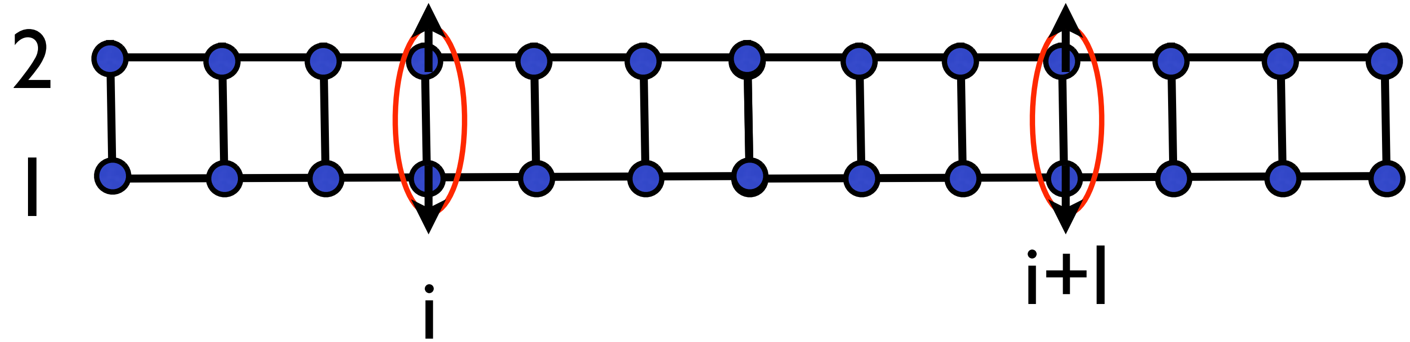
R.M.Noack et al ,PRL 1994



$\Delta_i^\dagger$ creates a singlet pair on rung i

$$\Delta_i^\dagger = \left(c^\dagger_{i,1\uparrow} c^\dagger_{i,2\downarrow} - c^\dagger_{i,1\downarrow} c^\dagger_{i,2\uparrow}\right)$$

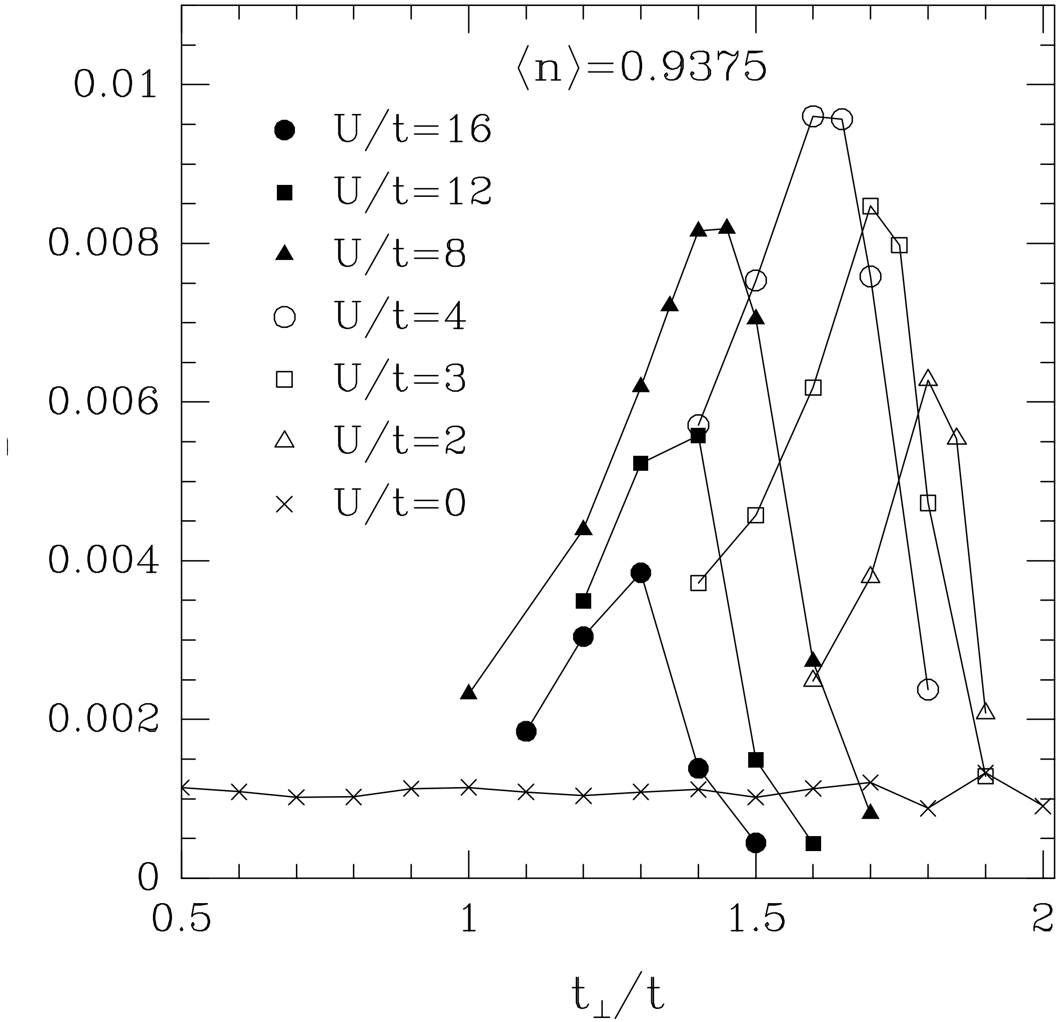
D is a measure of the strength of the pairing correlations.



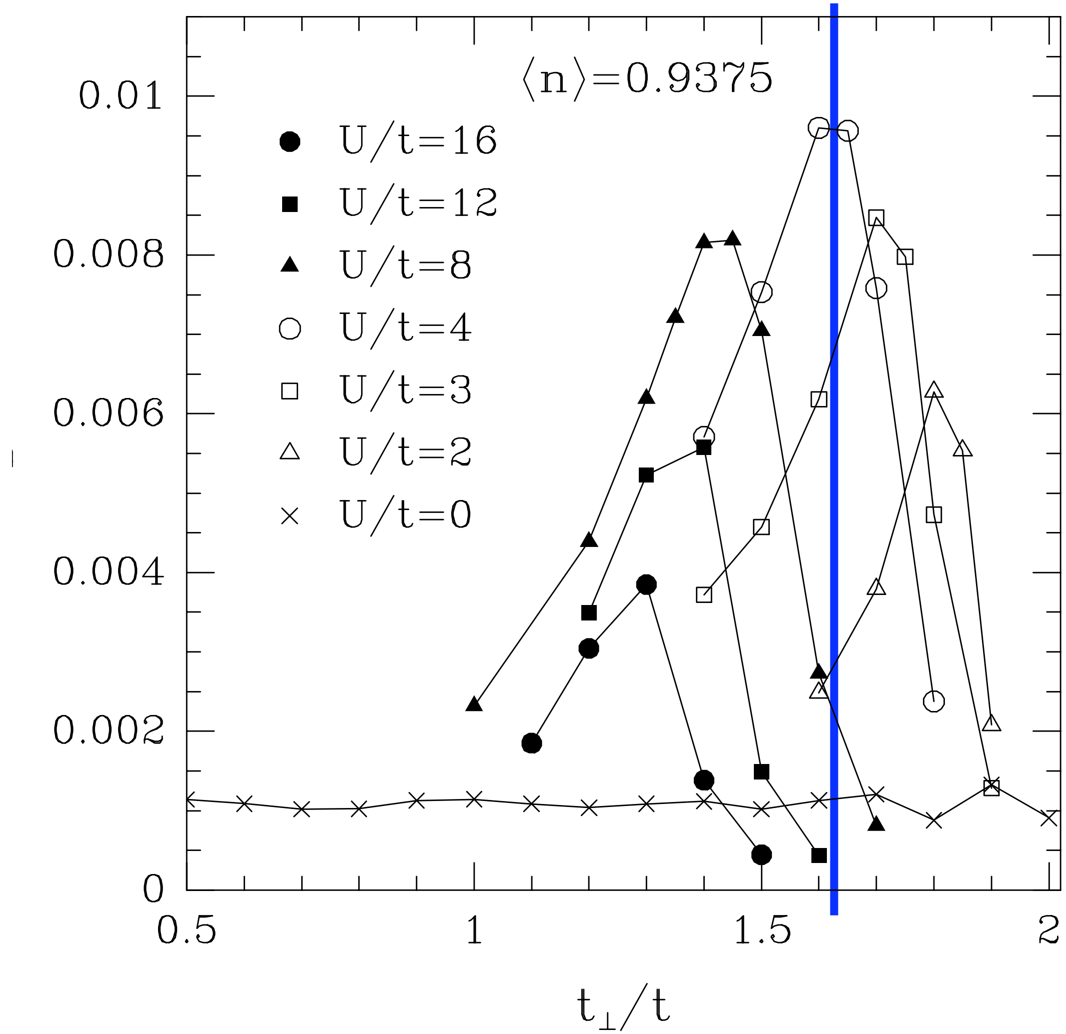
$\Delta_i^\dagger$ creates a singlet pair on rung i

$$\Delta_i^\dagger = \left(c_{i,1\uparrow}^\dagger c_{i,2\downarrow}^\dagger - c_{i,1\downarrow}^\dagger c_{i,2\uparrow}^\dagger\right)$$

$$D = \sum_{l=8-12} < \Delta_{i+l} \Delta_i^\dagger >$$



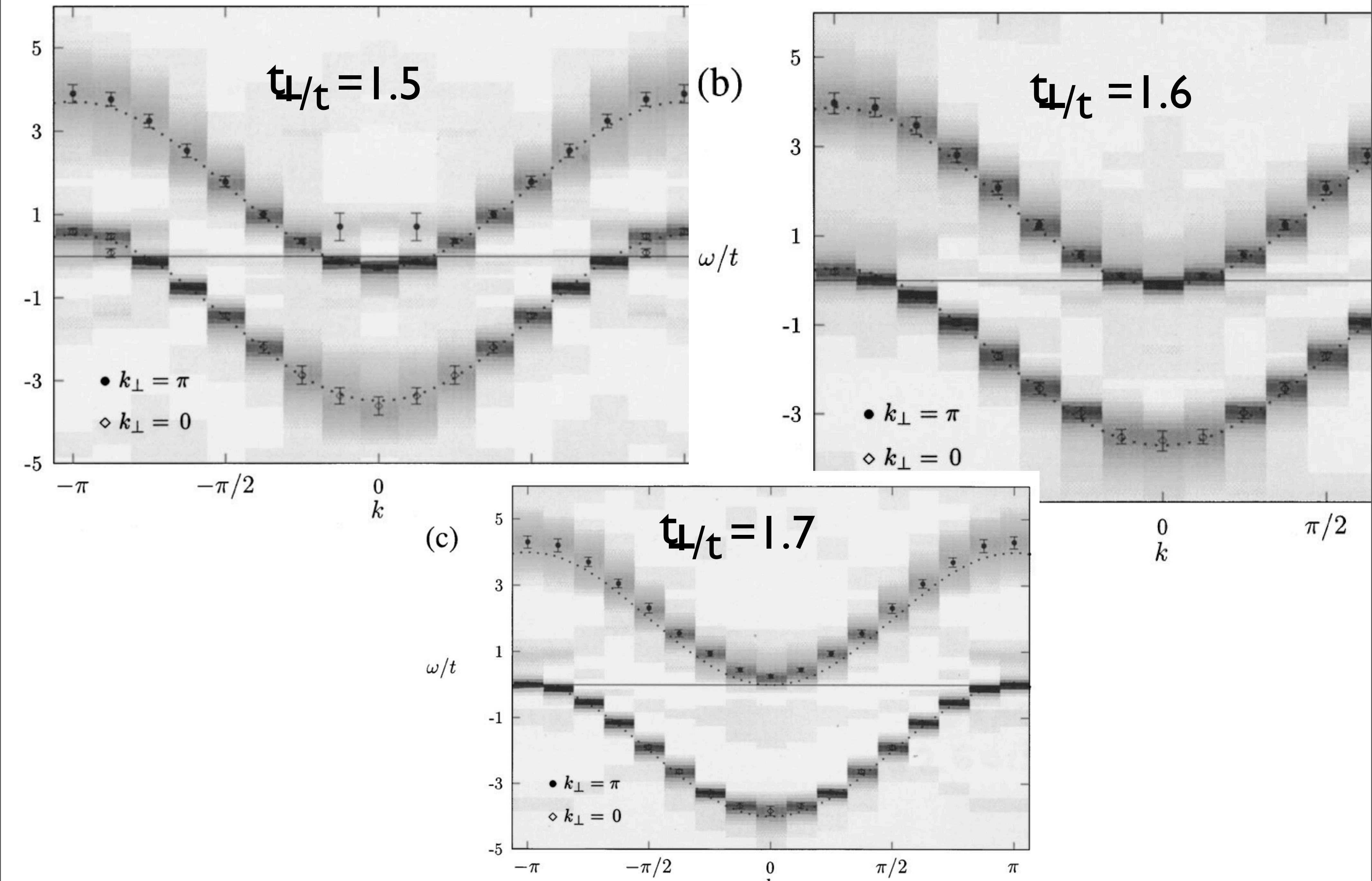
R.M.Noack et al PRB 56, 7162 (1997)



U/t=4

$t_{\perp}/t$ =1.62

R.M.Noack et al PRB 56, 7162 (1997)


t⊥/t =1.5
(b)
t⊥/t =1.6
(c)
t⊥/t =1.7
ω/t
k
5
3
1
-1
-3
-5
−π
−π/2
0
π/2
π
● k⊥ = π
◇ k⊥ = 0

Fine tuning

The pairing response of the 2-leg ladder can be enhanced by varying $t_\perp/t$ and <n>.

So, there are some problems and questions that still remain and whose solutions may lead to higher temperature superconductivity.

Competition with CDW and Peierls phases, and striped phases

Strength of the coupling g

Retardation

Negative U centers

Structure and microstructure