• d-RVB Phases in 1- and 2-Dimensions

T.M.Rice, ETH Zürich

- Strong Coupling Phases extrapolated from divergent RG-flows
- 1D test case: 2-Leg Ladder at $\frac{1}{2}$ -filling
  → d-RVB (d-Mott)
- 2D: RG-flow with Saddle Points close to E_F
  → d-RVB forms at high energies
  → d-Superconductor at low energies

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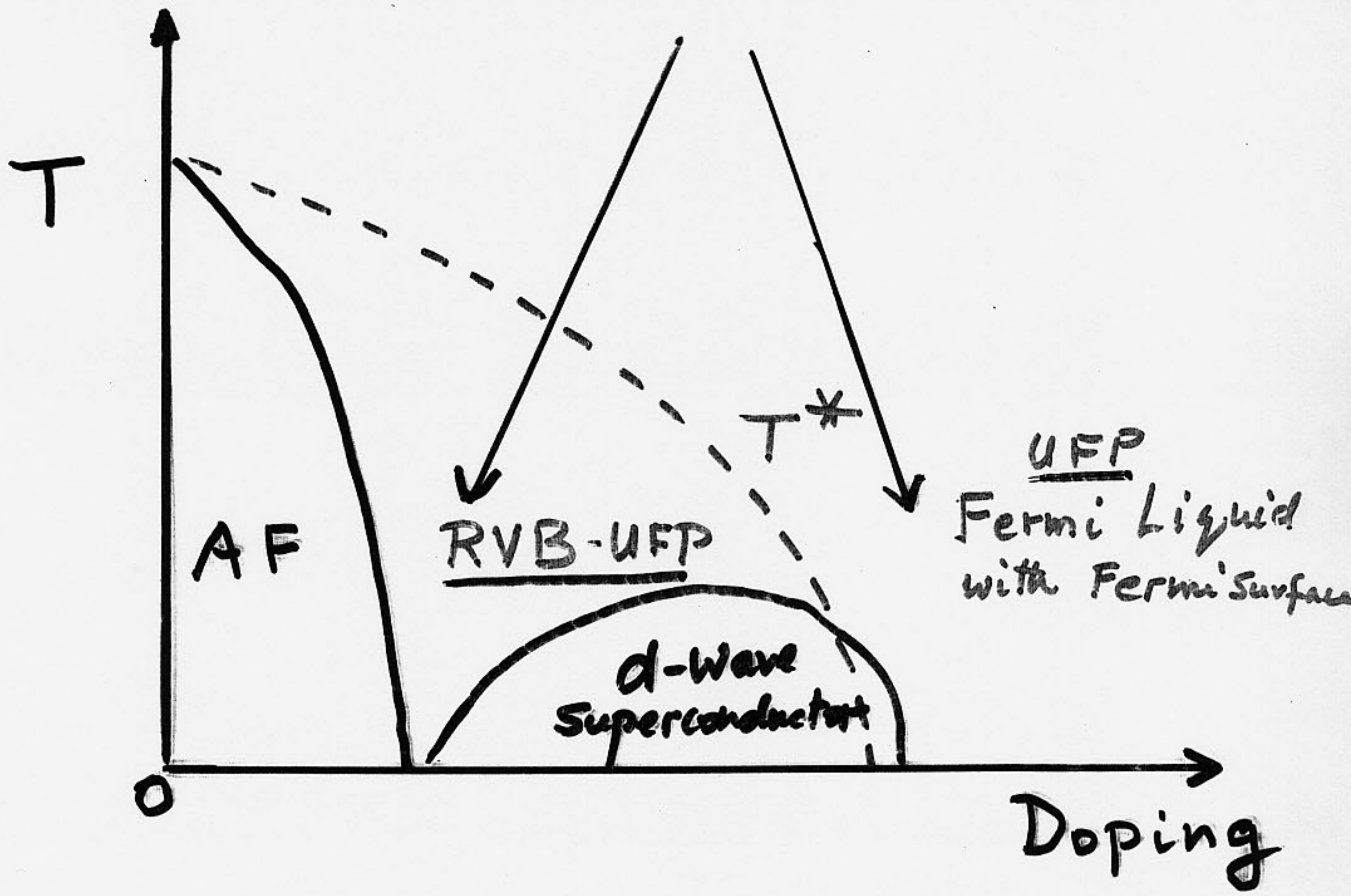
Carsten Honerkamp, MPI, Stuttgart

· cond-mat 0309567

· PRL '04

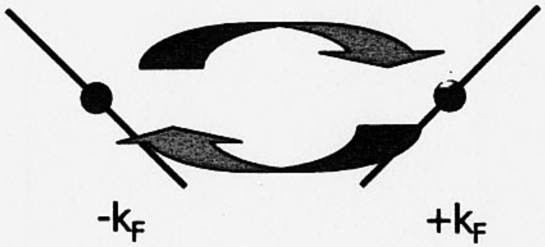
High-Tc Phase Diagram



see P. W. Anderson Physica B 2002

- "In praise of unstable fixed points: [UFP]
the way things actually work"

Introduction



Succesful approach in one dimensional electron systems:

1. perturbative RG
2. bosonization of the low energy Hamiltonian
3. field-theoretical analysis of the bosonized theory

What can we do if bosonization is not possible,
as e.g. in two dimensional systems ?
$\Rightarrow$ Numerical analysis of RG Hamiltonian

Fermions with an attractive interaction

1-Loop RG

$\Lambda-$Scale

$$\longrightarrow \quad g(\Lambda)=\frac{g_0}{\ln(\Lambda/\Lambda_0)} \xrightarrow[\Lambda\to\Lambda_0]{} -\infty$$

⇒ $\Lambda<\Lambda_0$: Mean Field Theory (BCS)

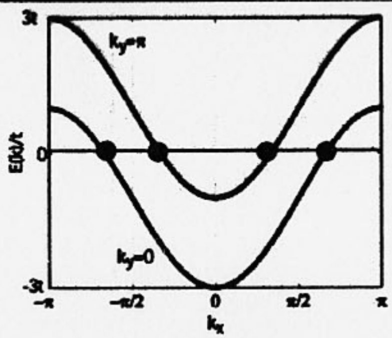
Equivalent to exact solution of

$$H^{\mathrm{BCS}}_{\mathrm{Red.}} = \sum_{\vec{k}\sigma} \varepsilon(\vec{k})\, c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma} + g \sum_{\substack{k_1,\sigma \\ k_2,\sigma'}} c^{\dagger}_{\vec{k}_1,\sigma} c^{\dagger}_{-\vec{k}_1,-\sigma} c_{\vec{k}_2,\sigma'} c_{-\vec{k}_2,-\sigma'}$$

⇓

Divergent Processes
in RG-flow

The half-filled two leg Hubbard ladder: RG-flow for initial U>0



RG Eqns.: $\dfrac{dg_i}{d\ell} = A_{ijk}\, g_j\, g_k$

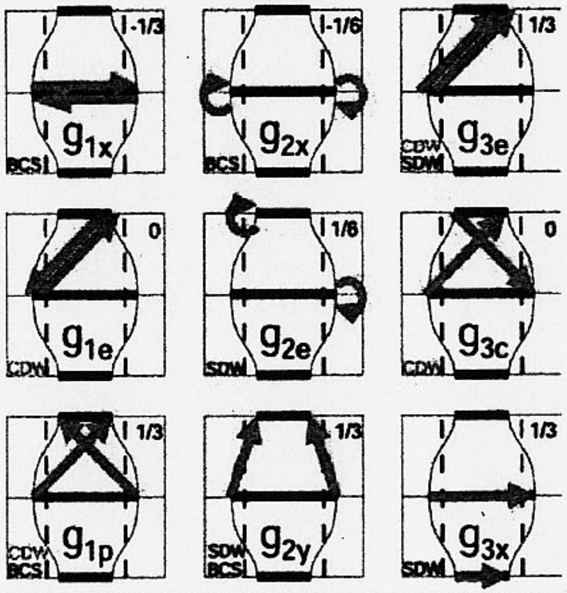
for generic repulsive interactions we flow towards a fixed ray in the interaction space
⇒ D-Mott phase (Lin, Balents, Fisher)
(d RVB)

g-ology

$k_y = \pi$

0

$-\pi$



Asymptotic flow:

$$g^0_{3e} = g^0_{3x} = g^0_{2y} = g^0_{1p} = -g^0_{1x} = \frac{1}{3} g^0_0$$

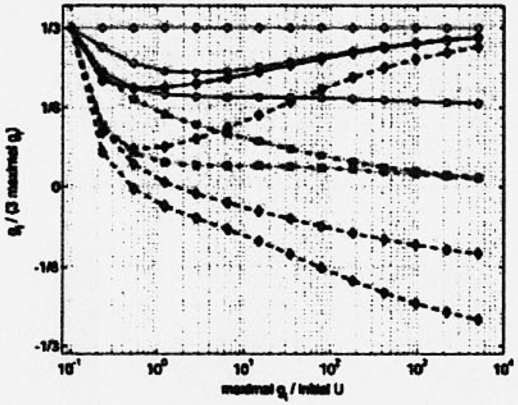
$$g^0_{2e} = -g^0_{2x} = \frac{1}{6} g^0_0, \qquad g^0_{3c} = g^0_{1e} = 0$$

with a logarithmic divergence:

$$g_i(\Lambda) = \frac{g^0_i}{\log(\Lambda/\Lambda_c)}$$

• A. Läuchli, C. Honerkamp, T.M.R.

Numerical Scheme



1. Given the RG-Equations, integrate them in order to obtain the asymptotic flow

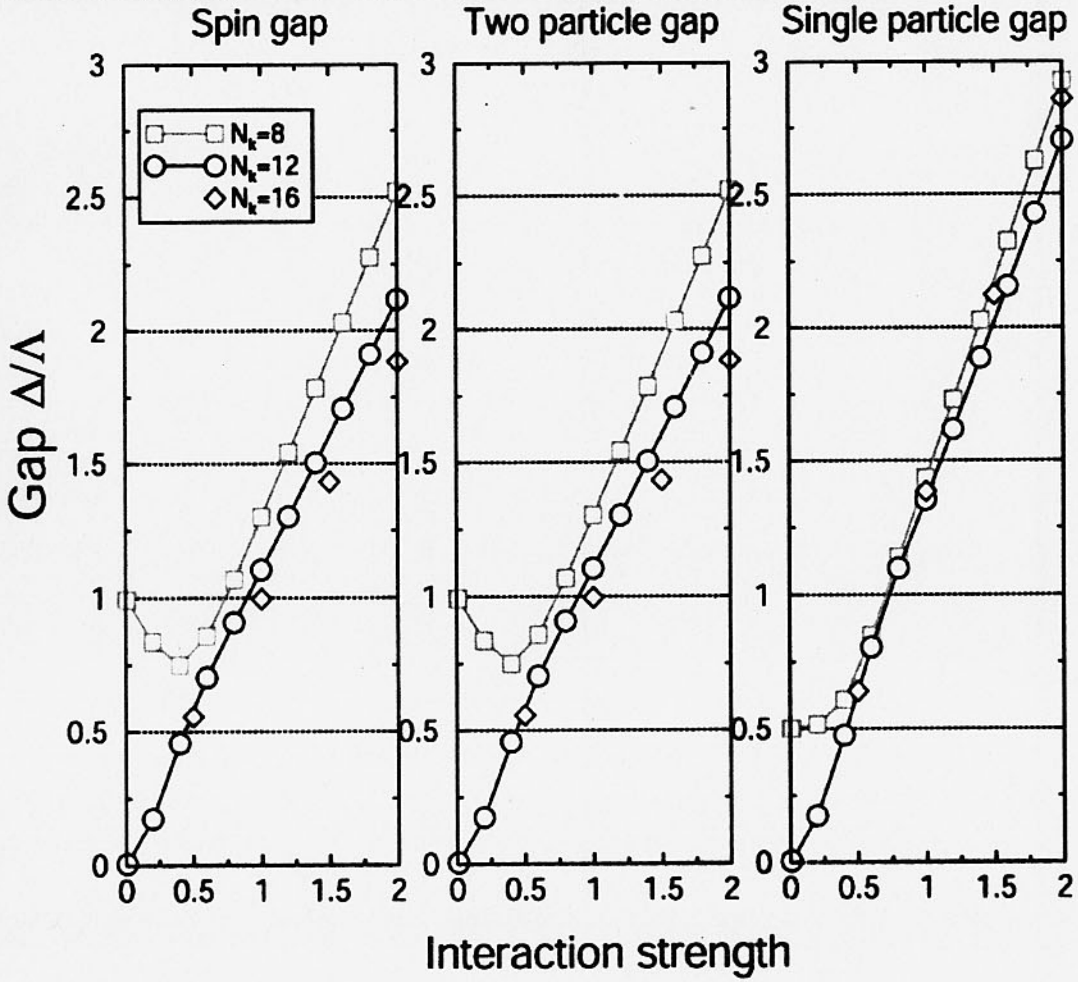
2. Translate the asymptotic RG-couplings to a Hamiltonian on a mesh in k-space. (λ =interaction strength parameter)

$$H=\sum_{k,\sigma}\varepsilon(k)n_{k,\sigma}+\lambda\sum_{\substack{k_1,k_2,k_3\\ \sigma,\sigma'}}V(k_1,k_2,k_3)\ c^{+}_{k_3,\sigma}c^{+}_{k_4,\sigma'}c_{k_2,\sigma'}c_{k_1,\sigma}$$

3. Perform an Exact Diagonalization of the resulting Hamiltonian for different number of k-points (up to 16 k-points feasible)

4. Calculate gaps and correlation functions (dynamics possible as well)
5. Perform finite size scaling

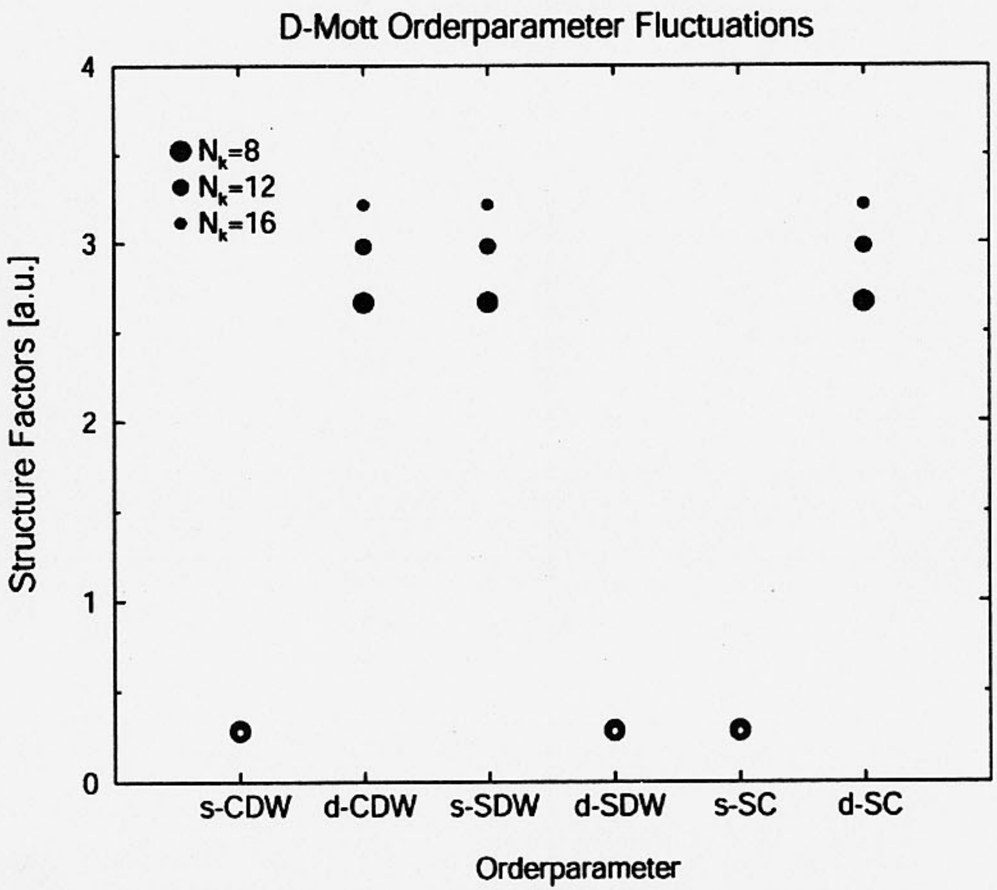
The half-filled two leg Hubbard ladder: Gaps in the D-Mott phase (dRVB)



- All gaps remain finite upon extropolating in $1/N_k$
- Bosonization predicts equal gaps in each channel [SO(8) symmetry]. This is approximately fulfilled in our finite size samples.
- $\Delta_s = E_G(N_0, S=1) - E_G(N_0, S=0)$
- $\Delta_{2p} = \frac{1}{2}[E_G(N_0+2, 0) + E_G(N_0-2, 0)] - E_G(N_0 0)$
- $\Delta_{1p} = \frac{1}{2}[E_G(N_0+1, \frac{1}{2}) + E_G(N_0-1, \frac{1}{2})] - E_G(N_0, 0)$

The half-filled two leg Hubbard ladder: D-Mott Orderparameters

d RVB



The groundstate of the repulsive Hubbard ladder at half-filling:

- Equally enhanced:
  - d-wave SC
  - SDW
  - d-Density wave
- But only SRO

$$O_{j\text{-}CDW} = \frac{1}{\sqrt{N_k}} \sum_{k,\sigma} f_j(k)\, c^{+}_{k,\sigma}\, c_{k+Q,\sigma}$$

$$O_{j\text{-}SDW} = \frac{1}{\sqrt{N_k}} \sum_{k,\sigma} f_j(k)\, \frac{\sigma}{2}\, c^{+}_{k\sigma}\, c_{k+Q,\sigma}$$

$$O_{j\text{-}SC} = \frac{1}{\sqrt{N_k}} \sum_{k,\sigma} f_j(k)\, c^{+}_{k\sigma}\, c^{+}_{-k,-\sigma}$$

$Q = (\pi, \pi)$

Form Factors: $f_s(k) = 1$; $f_d(k) = (\cos k_x - \cos k_y)/c$

The half-filled two leg ladder: 4 dominant phases

Lin, Balents, Fisher ′98; Fjaerestad, Marston ′01

In the half-filled two leg ladder there are four dominant phases at weak coupling:

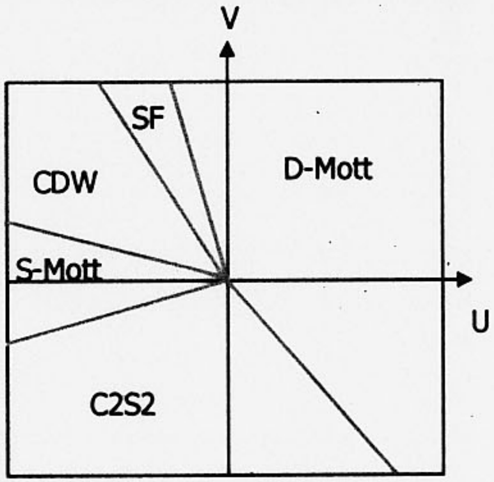
Phases realized in the SO(5) SZH model

D-Mott

SRO
d-SC
(π,π) s-SDW

Staggered Flux / d-CDW

LRO
(π,π) d-CDW
Symmetry broken



J=4(U+V)
weak coupling
phase diagram

S-Mott

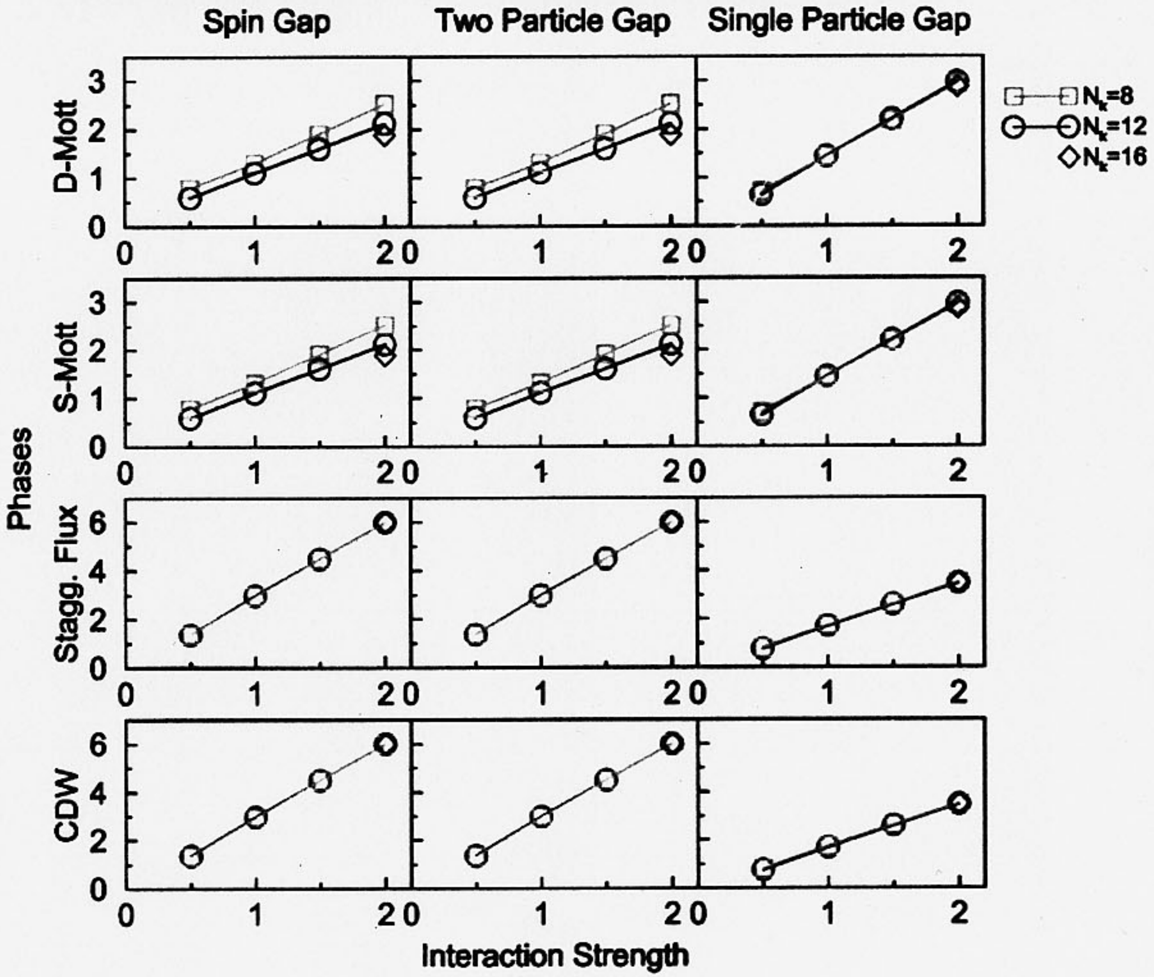
SRO
s-SC
(π,π) CDW

CDW

LRO
(π,π) CDW
Symmetry broken

The 4 dominant phases: Gaps

• A. Läuchli



D-Mott and S-Mott

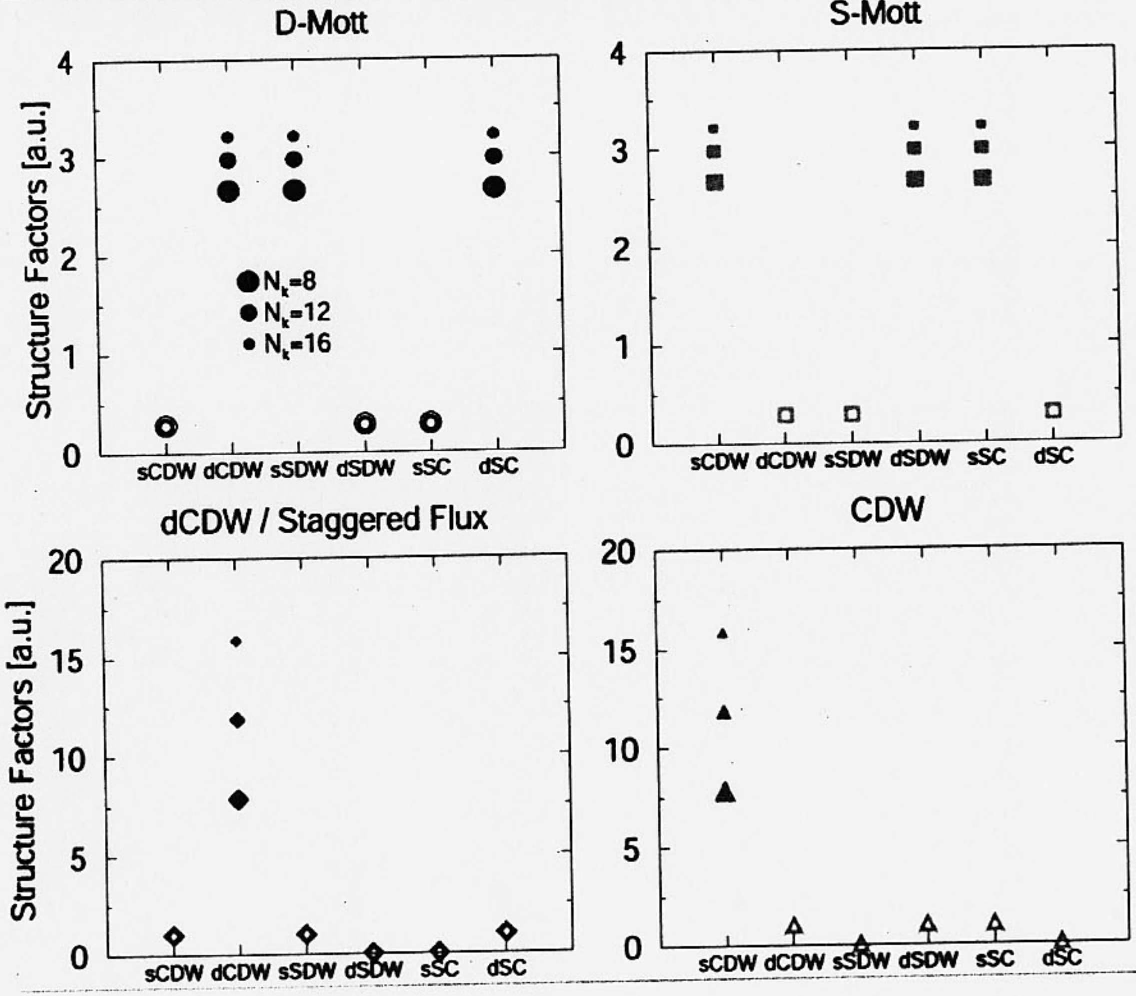
- finite size scaling of gaps indicate non-zero Gaps.
- nondegenerate GS
- only SRO

S.F. and CDW

- almost no finite size corrections
- degenerate GS
- true LRO

SO(5): equal spin and two particle charge gap.

The 4 dominant phases: Order-parameter Susceptibilities



D-Mott, S-Mott:

- insulating
- gaps to all excitations
- unique Groundstate
- short range ordered
- unbroken symmetry

Staggered Flux and CDW phases

- insulating
- gaps to all excitations
- 2-fold deg. groundstate
- long range ordered
- Z_2 symmetry broken

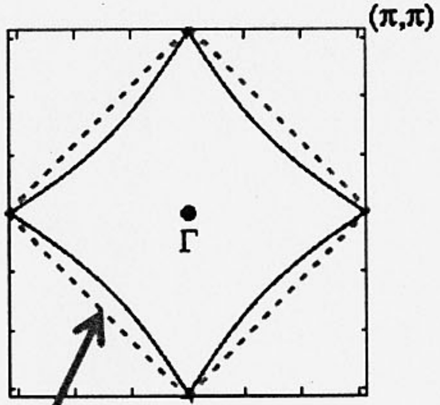
2 Dimensions. t-t'-U model

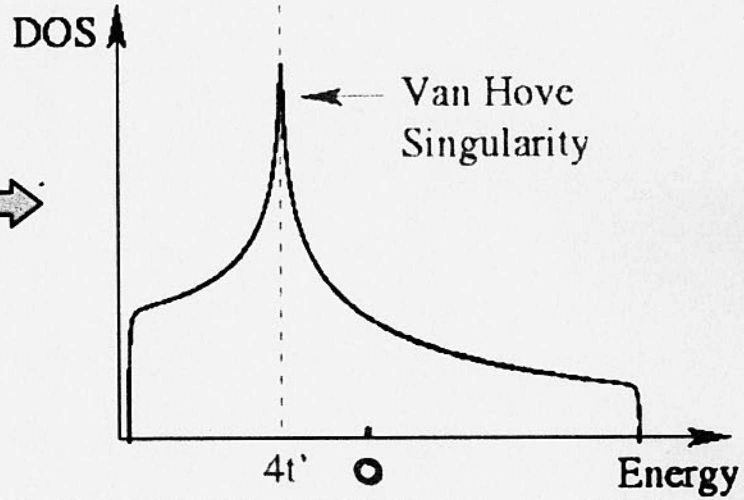
$$\varepsilon(\mathbf{k}) = -2t[\cos(k_x) + \cos(k_y)] - 4t' \cos(k_x)\cos(k_y)$$

n.n. n.n.n. hopping

U: Hubbard Interaction: $U n_{i\uparrow} n_{i\downarrow}$

- - - - - - t' =0, μ =0





Van Hove density ⇒ When $\mu = 4t'$ Fermi Surface intersects saddle points $(0,\pm\pi)(\pm\pi,0)$

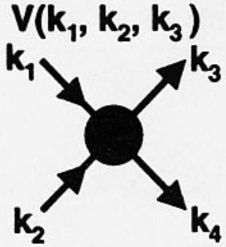
Possible Instabilities

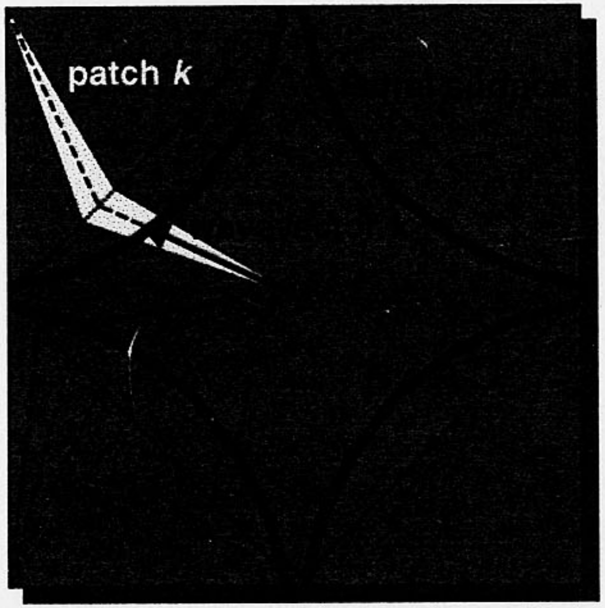
If

$|t'/t| \ll 1$ near to 1/2 -filling < AF: nesting, d-wave pairing

$|t'/t| \lesssim 1$ far from 1/2 -filling < F: stoner, p-wave pairing

Numerical implementation in 2D: The *N*-patch technique





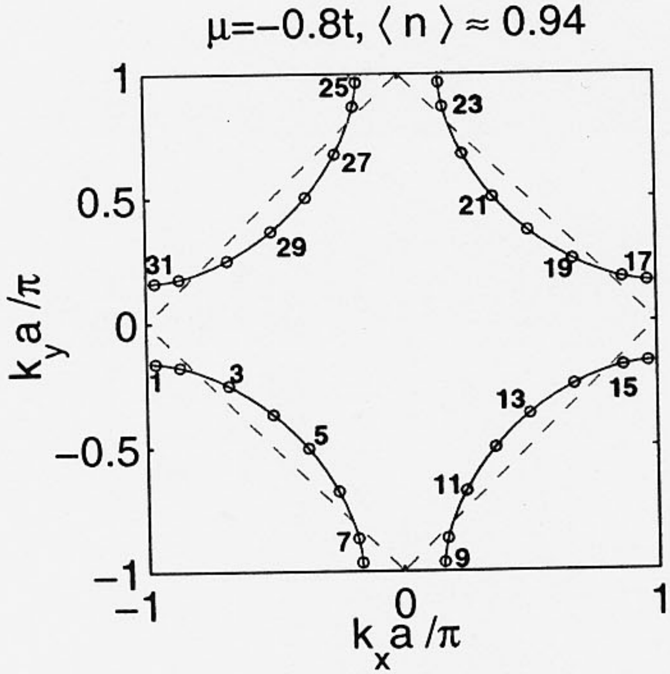
following **Zanchi and Schulz** 1997
Similar approaches:
Halboth& Metzner 2000,
Tsai& Marston 2001

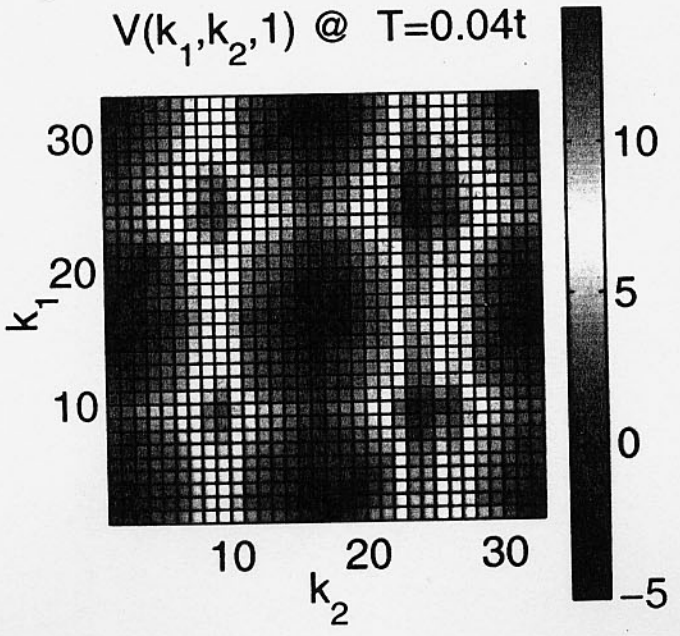
- Consider flow of couplings $\mathbf{V(k_1, k_2, k_3)}$ with incoming wavevectors $\mathbf{k_1, k_2}$ and 1st outgoing wavevector $\mathbf{k_3}$ **on the FS**, $\mathbf{k_4}$ is **fixed** by momentum conservation.
- take $\mathbf{V(k_1, k_2, k_3)}$ **constant** for all $\mathbf{k_1, k_2}$ and $\mathbf{k_3}$ in **same patches**.
- **neglect frequency dependence** of couplings.
- all phase space integrals are done as sums of radial integrals along the lines:

$$\int d^2k \quad \rightarrow \quad \sum_{k=1}^{N} w(k) \int dr\, r$$

- we calculate with patch numbers from N =32 to 144.

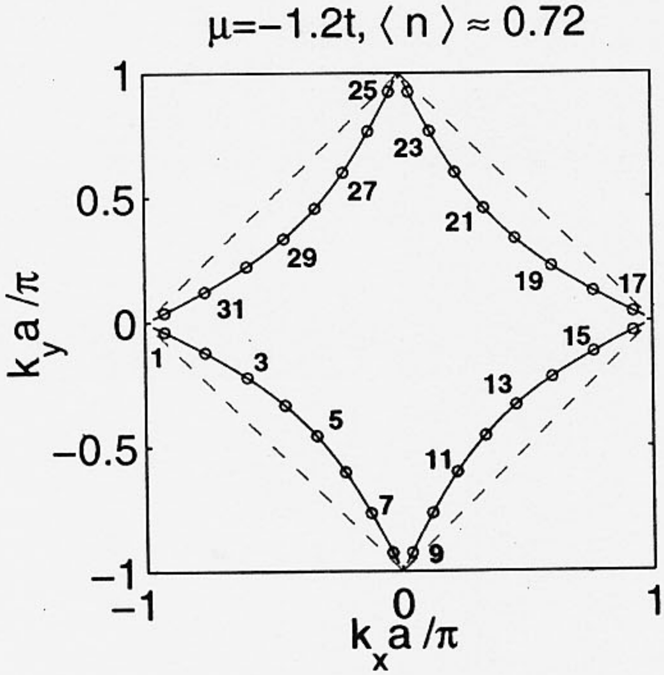
Close to Half-Filling; "Approximate Nesting"





- Umklapp Processes Dominate

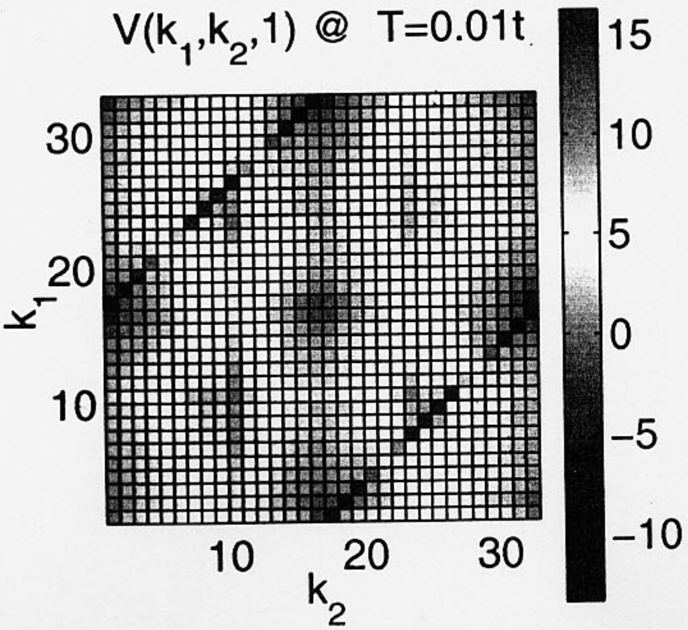
• **Low Electron Density**; "d-wave dominated"



· starting
· parameters

$t' = 0.3t$

$U = 3t$



Interactions

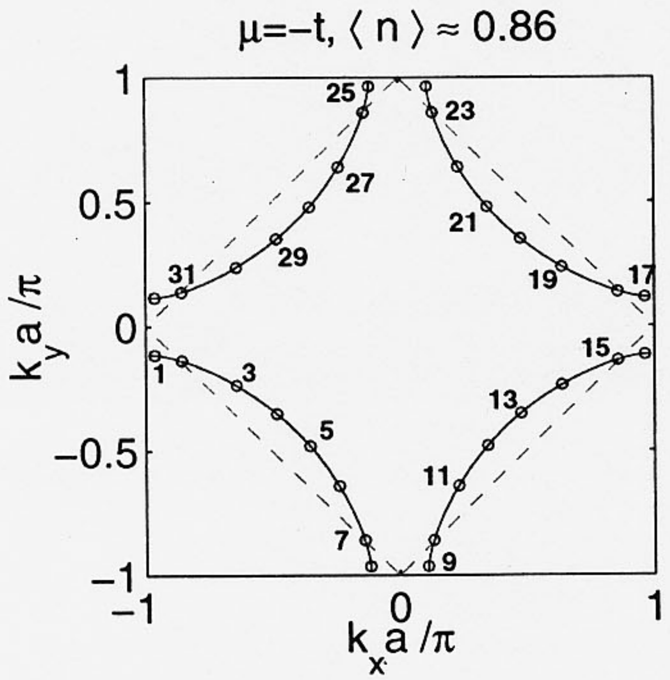
$V(k_1, k_2, k_3, k_4)$

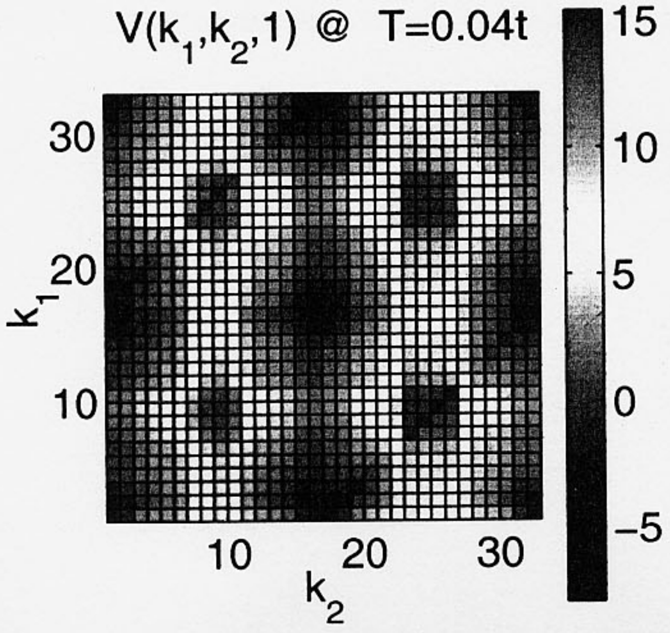
with $k_3 = 1$

$k_3 + k_4 = k_1 + k_2$: mod (G)

• d-wave Cooper pairing

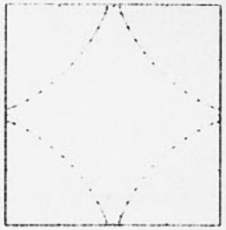
· Intermediate Density ; "Saddle Points"



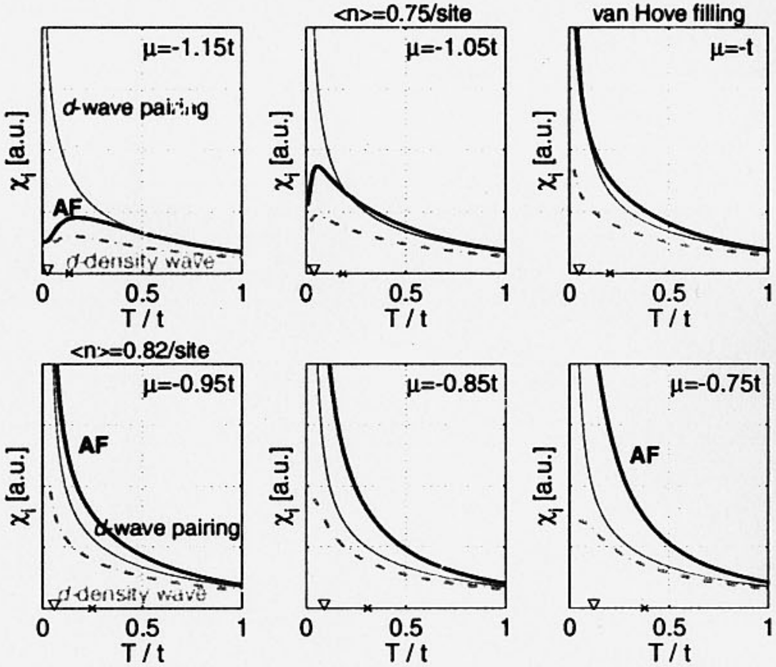


Pairing + Umklapp processes

$t' \approx -0.25t$: the saddle point regime



- Vary band filling around the van Hove value at fixed $t'=-0.25t$, initial $U=3t$.
- **Filling smaller than saddle point filling** ($\mu > -t$): only **d-wave pairing** channel singular at low T.
- **Filling slightly larger than saddle point filling** ($\mu \leq -t$): several channels grow togther driven by scattering processes between the saddle points: the **saddle-point regime**
  - ➔ **d-wave pairing** and **AF** susceptibility grow comparably in the range of validity
  - ➔ orbital AF (sF,DDW) grows as well (but not leading instability)
  - ➔ **Charge compressibility** suppressed (most strongly at saddle points)



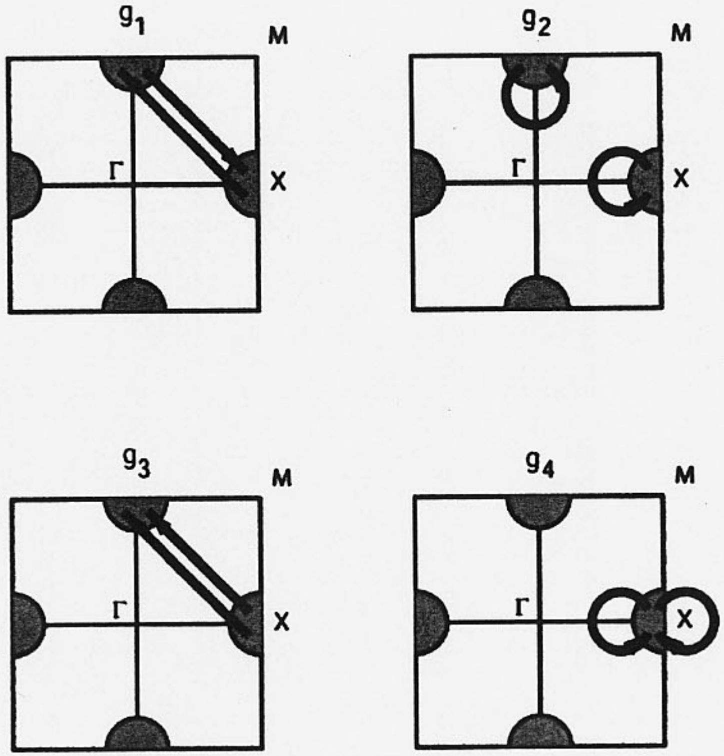
Mutual reinforcement of **d-wave pairing** and **AF** channel: both channels driven by same scattering processes between the saddle points.

Honerkamp, Rice, Salmhofer '02

Two patch approach to the 2D t-t' Hubbard model

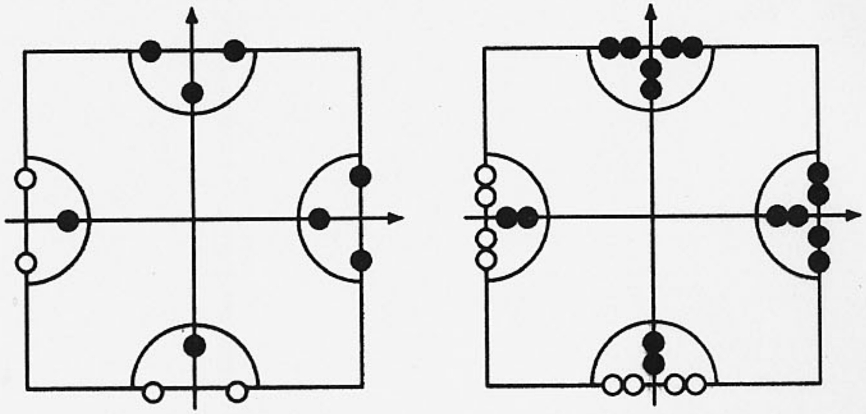
Interaction vertices
for the two patch model: $g_1,..,g_4$

Lederer, Montambaux, Poilblanc ('87)
Furukawa, Rice, Salmhofer ('98)

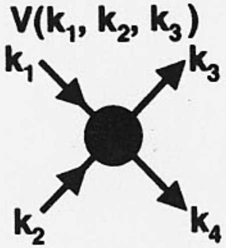


RG, repulsive U $\Rightarrow$ $g_1=0$, $g_2=1$, $g_3=2.2$, $g_4=-1$

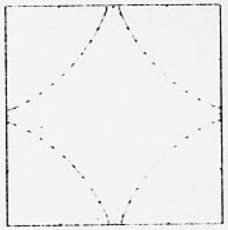
Discretization scheme:



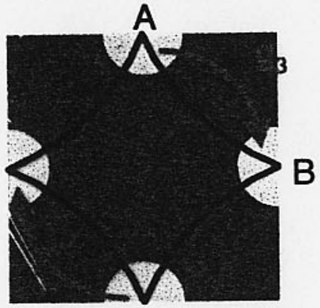
8 k-points   16 k-points



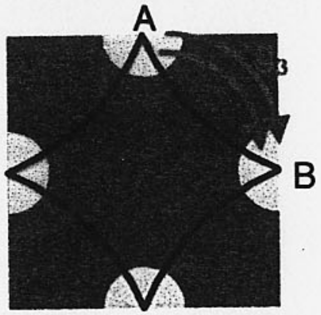
Cooper and Umklapp processes at the saddle points



Cooper process:
zero pair momentum



Umklapp process:
(π,π) momentum transfer



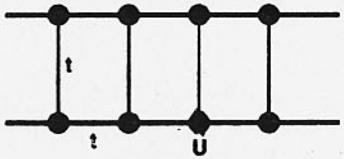
- **Cooper** couplings **drive d-wave pairing** fluctuations through particle-particle channel
- **Umklapp processes** drive **antiferromagnetic** and other (π,π)–fluctuations through particle-hole channel
- in one-dimensional systems: Umklapp scattering causes Mott **charge gap**
- in one-loop RG: Umklapp processes suppress charge compressibility

Fermi surface near saddle points: (π,π)–Umklapp processes have almost zero pair momentum: **mutual reinforcement** of **d-wave pairing** and **AF**-(π,π)-channel, both channels driven by same scattering processes between the saddle points.

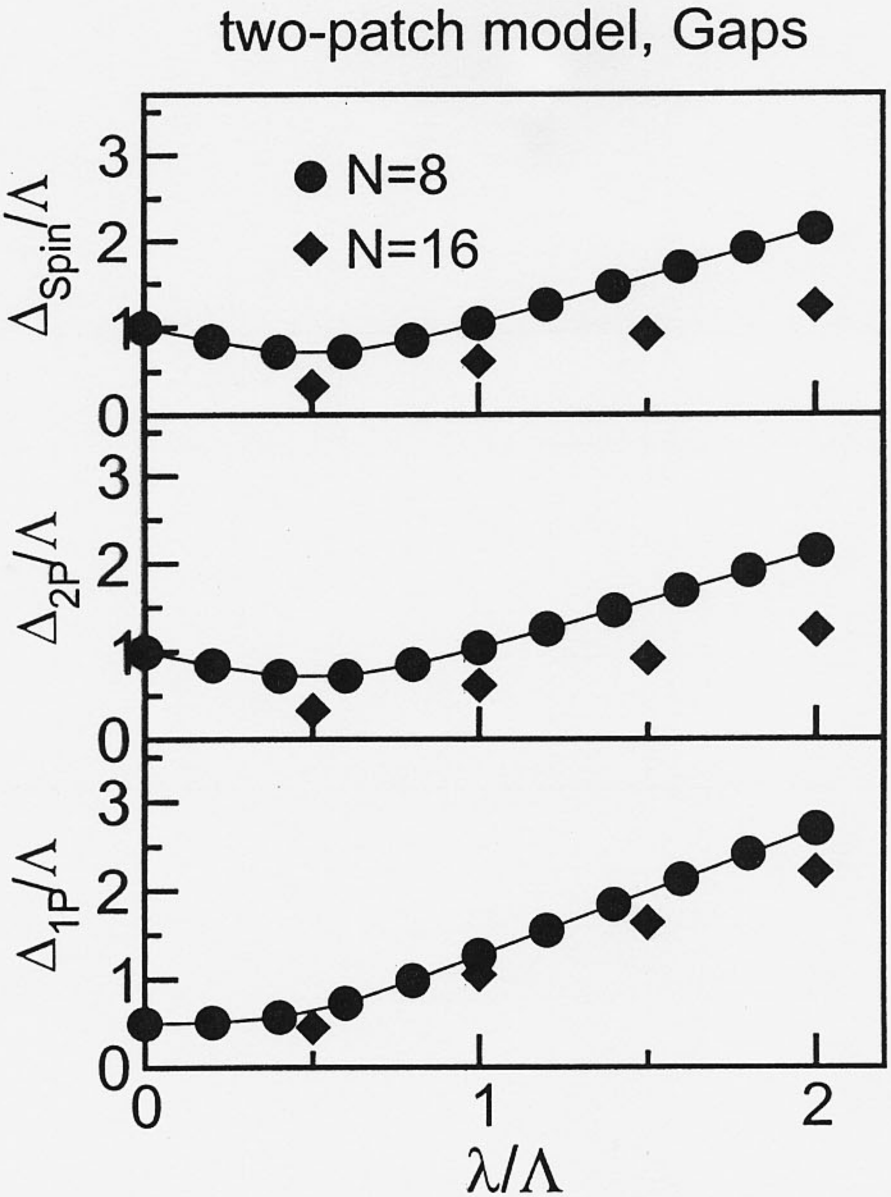
What is the strong coupling state in the saddle point regime ?

- Flow to strong coupling in the **half-filled two-leg Hubbard ladder**:
  - ➔ **d-wave pairing**, **AF** and **orbital AF** susceptibilities diverge with same exponent, **charge compressibility** suppressed
  - ➔ Bosonization (Lin, Balents& Fisher 1998), DMRG (Noack 1994):

    Strong coupling state is **insulating spin liquid** (ISL) **without long range order**, with spin and charge gap.



- RG flow at saddle points in 2D model qualitatively similar to half-filled two-leg Hubbard ladder (Furukawa,Rice 1998, Honerkamp,Salmhofer,Rice 2001)
  - ➔ Analogous **strong coupling state** at the saddle points?
  - ➔ **d-wave pairing, antiferromagnetic** and **orbital AF (sF,DDW)** correlations embodied as **short range correlations**? (→*t-J* model, Ivanov et al. 1999)
  - ➔ BZ diagonals remain gapless ?

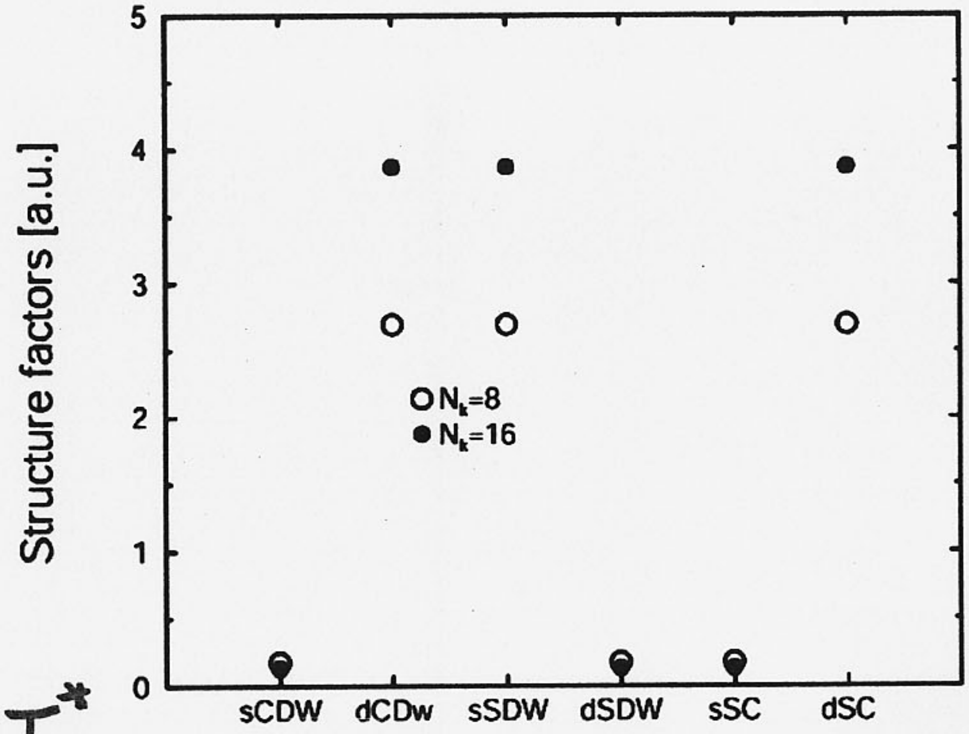

two-patch model, Gaps
N=8
N=16
Δ_Spin/Λ
Δ_2P/Λ
Δ_1P/Λ
0
1
2
3
λ/Λ

Two patch approach to the 2D t-t′ Hubbard model

Order parameter susceptibilities reveal similarities to the D-Mott phase of the Hubbard ladder:

- equally enhanced:
    - d-CDW
    - s-SDW
    - d-SC
- but presumably SRO

→ d RVB at T^*



Doping of a 3–Leg Ladder

3 bands at E_F:	2 even	+	1 odd parity
	↓		↓
half–filling:			
1el/site charge:	gap		gap
spin:	gap		gapless
low doping, $\delta < \delta_c$:			↗ holes enter here

Fermi surface only in odd parity channel
even parity channel truncated by U–processes

➔ **Partial truncation of the Fermi surface**,
similar results for n–leg ladders *(Ledermann, LeHur, Rice)* PRB '00

3-Leg Ladder

OYA Theorem: Gapless Excitations at a
[Generalization of LSM Theorem]
wavevector: $2\pi . 3 . \frac{1}{2}(1-\delta)$

$$= \underline{3\pi - 3\pi\delta}$$

δ: doping

Partially Truncated Fermi Surface has an gapless excitation in the Luttinger Liquid in the odd parity band

with wavevector : $\pi(1-3\delta)$

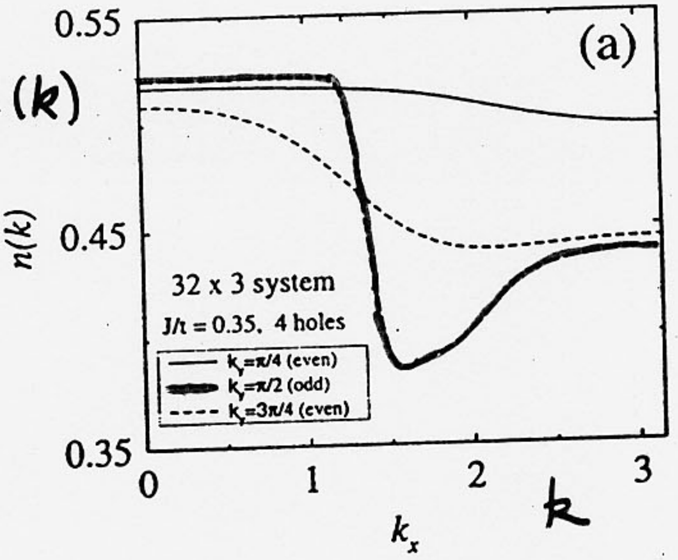
$$= \underline{\pi - 3\pi\delta}$$

$\Rightarrow$ Equivalent mod (2π)

Hole Doping of a 3-Leg Ladder

• Rice, Haas, Sigrist, Zhang
PRB '97

t-J model



DMRG

• White and Scalapino
PRB '98

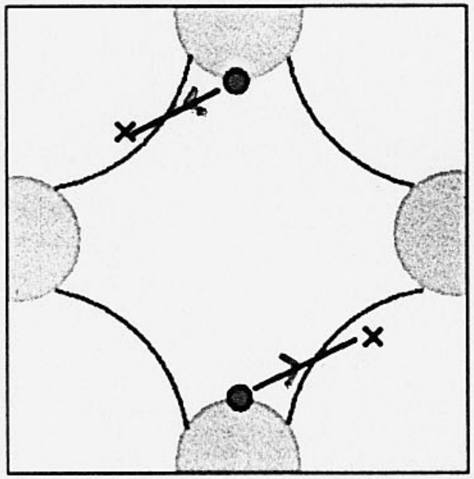
⇒ Fermi Surface only in odd parity band

→ holes enter only in odd parity band.

Low Energy Scale (T < T*)

Two Fluid Model

- Insulating Spin Liquid (d-RVB) at Saddle Points (S)
- Fermi Liquid Arcs near BZ diagonals (A)



Coupling via Cooper Process

Pariring Interaction induced on the Arcs

$$V_{AA} = -V_{AS}{}^{2}\chi_s^d \frac{T^3}{2\Omega}\sum_{\substack{k,k'\\ \sigma,\sigma'}} g_{\vec{k}}\, g_{\vec{k}'}\, c^{\dagger}_{\vec{k},\sigma} c^{\dagger}_{-\vec{k},-\sigma} c_{-\vec{k}',-\sigma'} c_{\vec{k}',\sigma'}$$

χ_s^d d-Wave pairing susceptibility → dSC

$$g_{\vec{k}} = \cos k_x - \cos k_y$$

Conclusions

- We have proposed a numerical method to analyze RG flows to strong coupling.
- The method is flexible and turned out to be useful for systems with pure SRO, quasi-LRO and true LRO.
- Its results are consistent with bosonization results.
- Since it is based on Exact Diagonalization we can calculate energy gaps, static and dynamical correlation functions directly in a fermionic description.