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XII WORKSHOP ON STRONGLY CORRELATED ELECTRON SYSTEMS

17 - 28 July 2000

D-WAVE SUPERCONDUCTIVITY FROM SUPEREXCHANGE INTERACTION

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D-wave superconductivity from **superexchange** interaction

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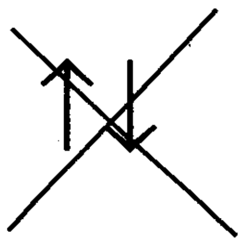
Recent results obtained with QMC:

- Lanczos algorithm with QMC
- Importance of a good variational guess
- Hole and spin Jastrow correlations
- d - wave superconductivity from J

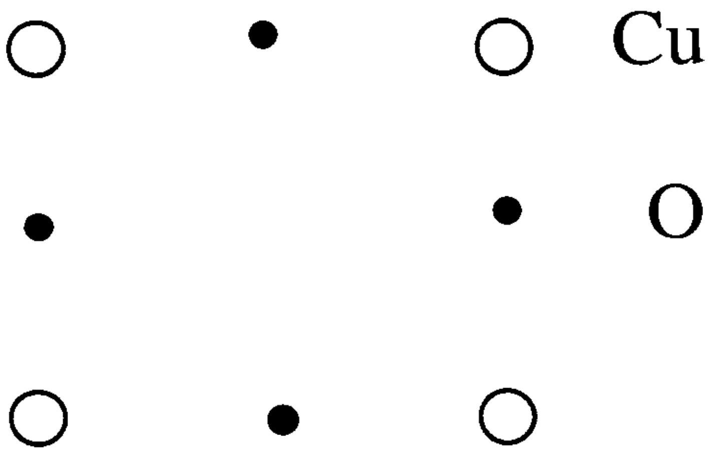
The t-J model

Phd Matteo Calandra
Federico Becca

$$H=\sum -t\, P c^{+}_{i\sigma} c_{j\sigma} P + h.c. + J\,(\vec{S}_i \vec{S}_j - \frac{1}{4} n_i n_j)$$



P → Strong correlation



Effective model of HTc (Zhang & Rice)
Hole → absence of spin in Cu sites

Lanczos algorithm: an efficient variational approach

Ground state $|\psi_{GS}\rangle$ of H approximated by using **p** variational parameters:

$$|\psi_{\mathbf{p}}\rangle = (1 + \alpha_1 H + \alpha_2 H^2 + \ldots \alpha_{\mathbf{p}} H^{\mathbf{p}}) |\psi_G\rangle$$

The $\{\alpha\}$ are determined by:

$$\mathrm{Min}\{\alpha\} \quad \frac{\langle \psi_{\mathbf{p}} | \mathrm{H} | \psi_{\mathbf{p}} \rangle}{\langle \psi_{\mathbf{p}} | \psi_{\mathbf{p}} \rangle}$$

Convergence $|\psi_{\mathbf{p}}\rangle \rightarrow |\psi_{GS}\rangle$ for **p** small

p~10 for <u>basically exact</u> $|\psi_0\rangle$

What can we do on large size ?

The power $H^{\mathbf{p}}|\psi_G\rangle$ are computationally demanding $L^{\mathbf{p}+1}$ operations $\Rightarrow$ very small **p**

L is the system size and/or electron number

We use the Stochastic Reconfiguration
S. Sorella, PRL (1998)
= & L. Capriotti PRB (2000)
=& F. Becca, M. Capone '' Lanczos ...

Lanczos +QMC

- an unbiased convergent algorithm: no freedom but the initial state $|\psi_G\rangle = |\psi_{p=0}\rangle$
- Correlation functions "easy" → no field

But **p=2** may appear very small

Variance error estimate

By increasing p $|\psi_p\rangle$ p = 0.1.2...

$$\left\| |\psi_p\rangle - |\psi_{GS}\rangle \right\| = \varepsilon_p \to 0$$

The energy $E_p = \langle \psi_p | H | \psi_p \rangle = E_{GS} + O(\varepsilon_p^2)$

Variance $\langle \psi_p | H^2 | \psi_p \rangle - \langle \psi_p | H | \psi_p \rangle^2 = O(\varepsilon_p^2)$

Thus linear behavior if $\varepsilon_p^2 << 1$

Numerical tests on a small 18 sites
Becca & al. cond-mat 0006353

It is amazing how good is the projected d-wave wf on a small size where the ground state is known

Tests at J/t=0.4:

$$Z = \left|\langle \psi_{\text{d-wave}} | \psi_{\text{EXACT}} \rangle\right|^2 = 0.93 \quad \text{2 holes}$$

$$= 0.83 \quad \text{0 holes}$$

The average sign of the wavefunction:

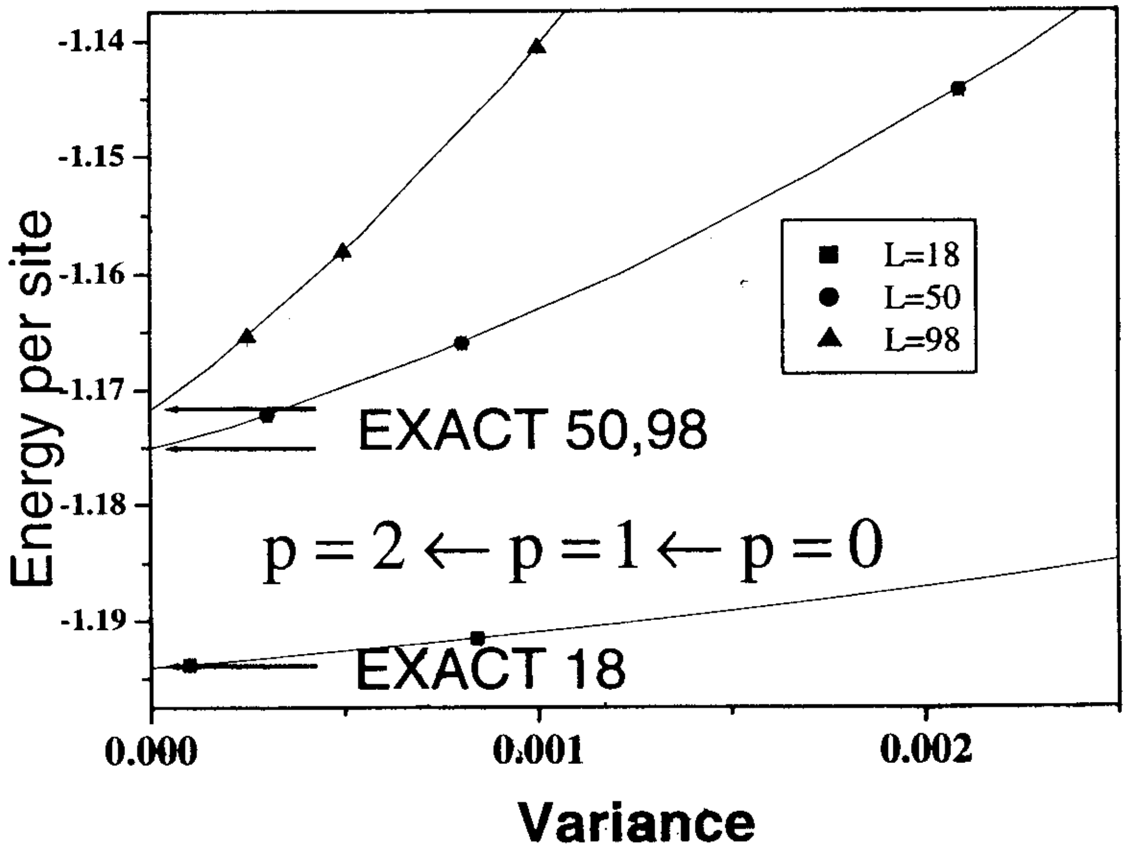
$$S = \sum_x \text{Sgn}(\psi_{\text{d-wave}}(x)\, \psi_{\text{EXACT}}(x))\, \psi_{\text{EXACT}}(x)^2 = 1 \qquad \text{0 holes}$$

$$= 0.99 \quad \text{2 holes}$$

Obviously with two Lanczos steps we get exact results Z>0.99

Variance extrapolation test

Heisenberg model AF long range order $\mathbf{m} = \mathbf{0.307}$
Initial "bad" $|\psi_{\mathbf{p=0}}\rangle = |\psi_G\rangle$ = BCS wf. with $\mathbf{m} = \mathbf{0}$
exact results known even for large # sites **L**



Exact energy results possible with p=0.1.2 variance extrapolation!

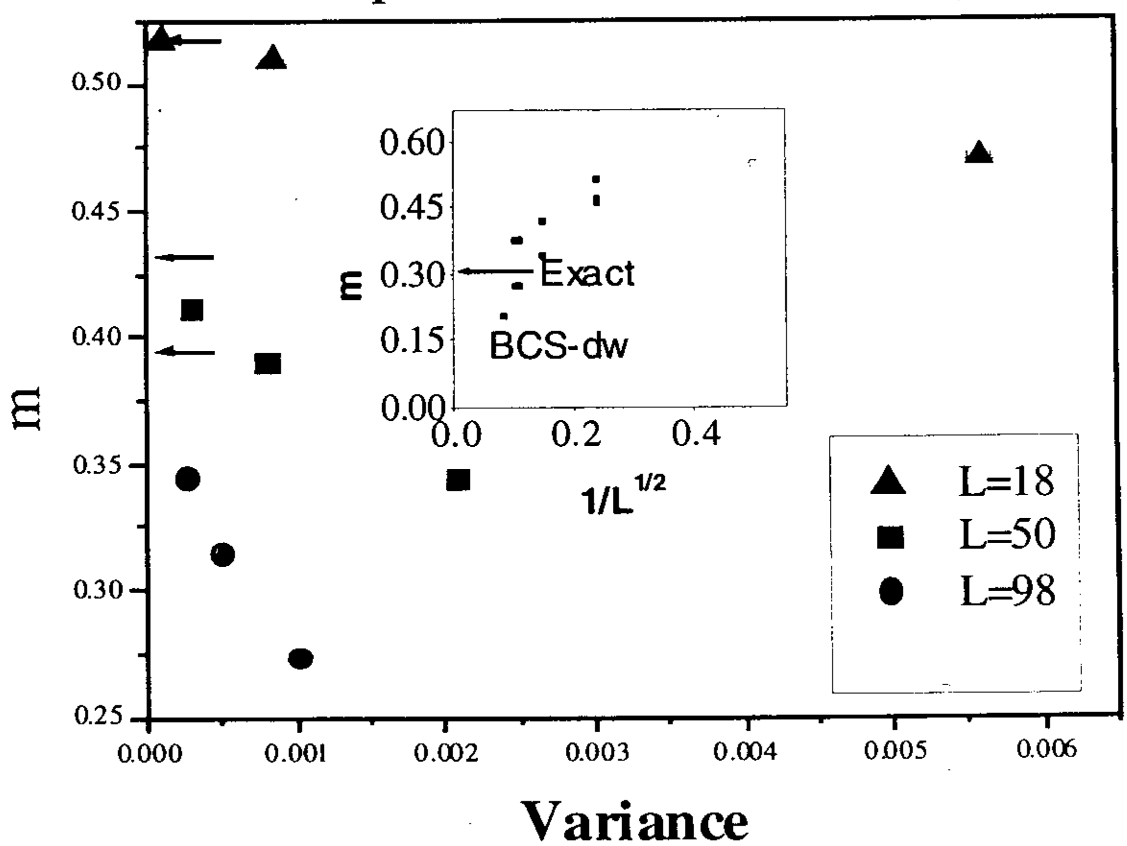
What about correlation functions ?

For operators O, estimated $\langle \psi_p | O | \psi_p \rangle$

Linear variance behavior if $[H, O] = 0$

In practice $[H, O] \cong 0$ for **most** interesting O

2 Lanczos step +BCS wf with Gutzw. projection



$$p = 2 \leftarrow p = 1 \leftarrow p = 0$$

Study of superconducting order

Probe directly the "anomalous" average:

$$P_d = \langle N+2 | \Delta^+ | N \rangle,$$

$|N\rangle$: the ground state with N particles on L sites

$\Delta^+ = 1/L \sum$ All possible d - wave n.n. singlet

[redacted]

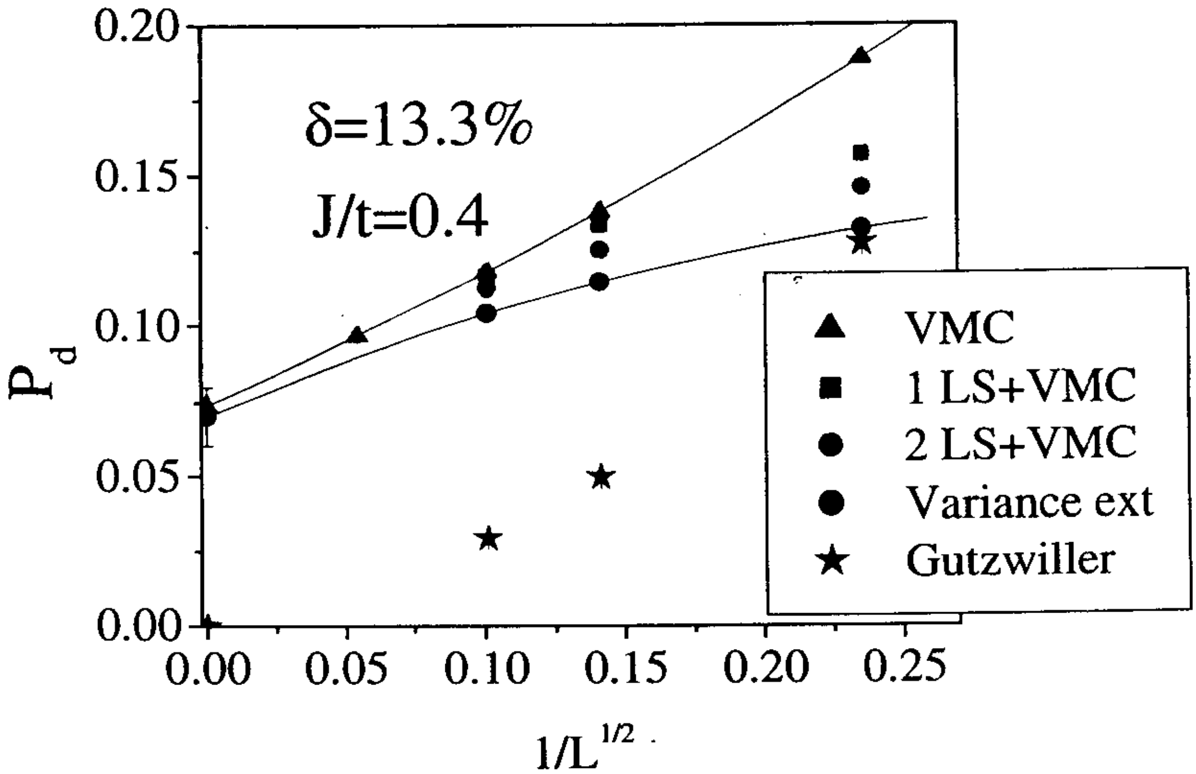
If there are no holes it is not possible to create singlets $\rightarrow P_d <\approx \delta$ (hole doping)

A very small signal proportional to δ and not to the # electrons is expected.

<u>But small does not mean zero...</u>

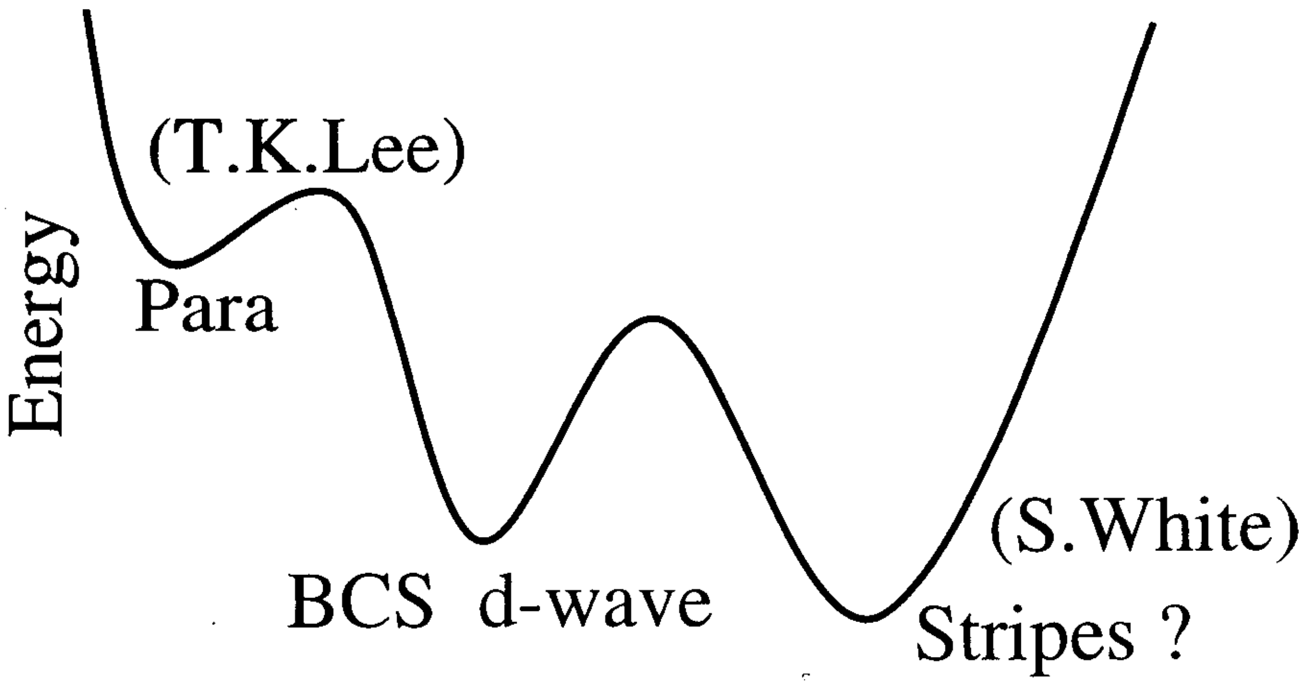
Finite size scaling in the t-J model

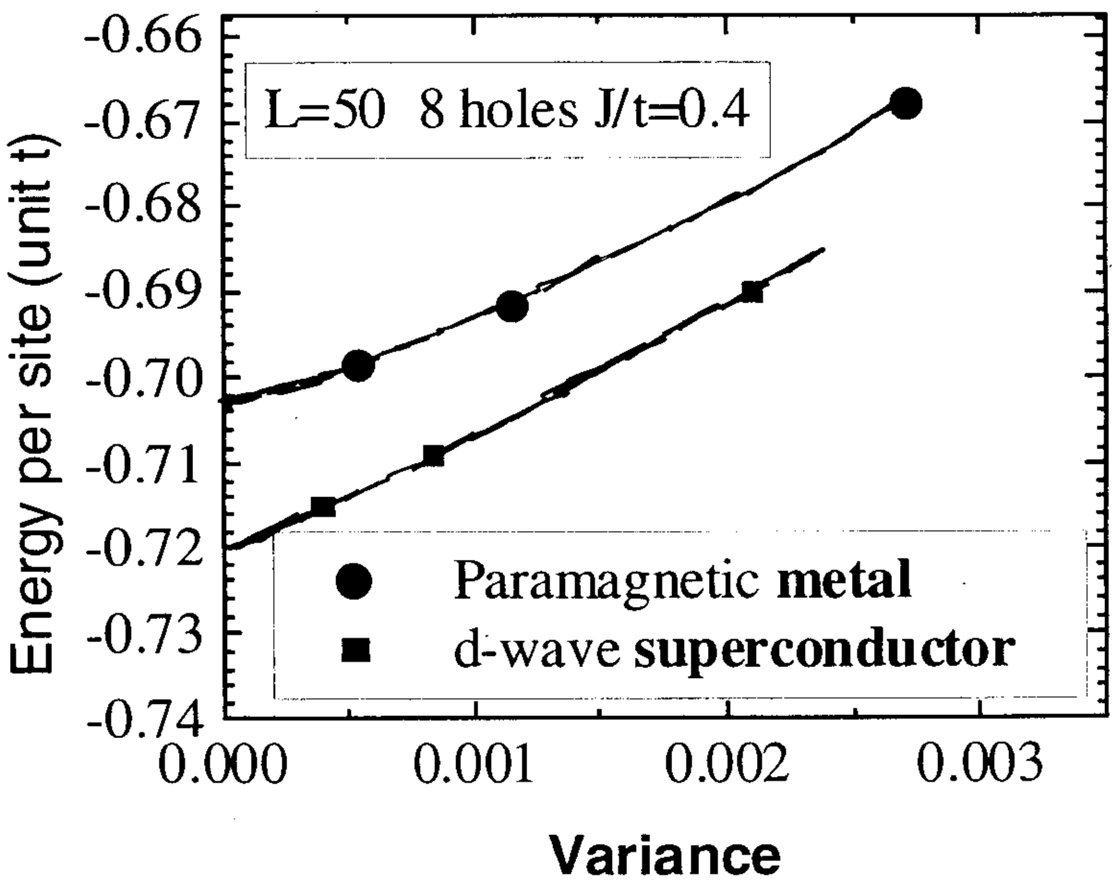
The drop of P_d is more evident for small sizes where a metal (Gutzwiller) ≈ superconductor



The effect is very clear: the 2D t-J model ground state has d-wave superconductivity

Finding the global mimimum state





The variational wavefunction

$$\psi_{VMC} = \exp(1/2 \sum_{R,R'} v_\rho(|R - R'|)\ n_R\, n_{R'} \quad \text{Hole - Jastrow}$$

$$\times \quad \exp(1/2 \sum_{R,R'} v_\sigma(|R - R'|)\ \sigma^z_R\, \sigma^z_{R'} \quad \text{Spin - Jastrow}$$

$$\times \quad |SD\rangle \quad \text{"Slater - determinant"}$$

$$H_{\text{ONE-BODY}} = \text{Free} + \sum_{R,\tau} \Delta(\tau)\,(c^+_{R,\uparrow} c^+_{R+\tau,\downarrow} + c^+_{R+\tau,\uparrow} c^+_{R,\downarrow}) + \text{h.c.}$$

$$+ \Delta_{AF} \sum_R (-1)^R\, (c^+_{R,\uparrow} c_{R,\uparrow} - c^+_{R,\downarrow} c_{R,\downarrow})$$

Δ_τ at any given distance $\|\tau\|$

reflection and rotation symmetry: e.g. $d_{x^2-y^2}$ (d - wave)

$\Delta_{AF} = 0$ for translation invariance satisfied

For a certainly singlet wavefunction:

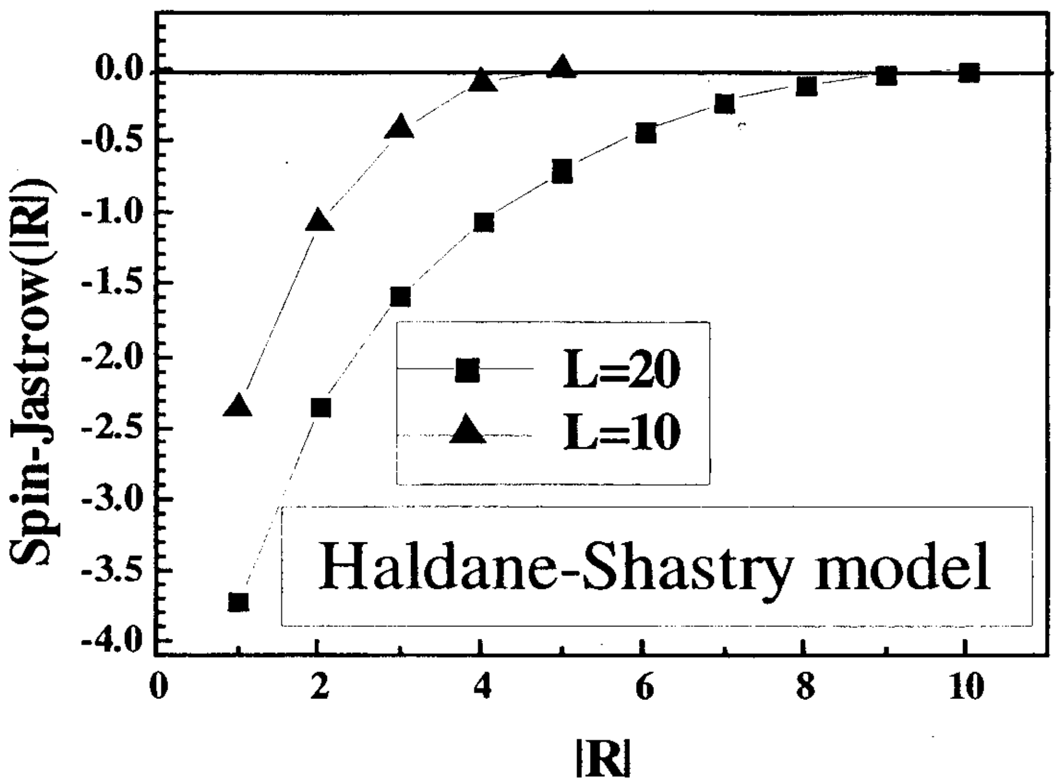
$$\boxed{v_\sigma = 0 \qquad \Delta_{AF} = 0}$$

Example 1D Haldane-Shastry model

$$H = \sum_{<R,R'>} J(|R-R'|)\ \vec{S}_R \bullet \vec{S}_{R'} \qquad J \propto 1/R^2$$

F.Franjic & S.S. Prog. Theor. Phys. '97

$$|\mathrm{SD}\rangle = \prod_{i\ \mathrm{even}} |\leftarrow\rangle \prod_{i\ \mathrm{odd}} |\rightarrow\rangle$$



This is the **exact** solution of the model

An RVB wavefunction at half filling when the Jastrow acts on the BCS state

Jastrow = Projector on no doubly occupied sites
& Fixed number of particles N = # sites

P.W. Anderson ('89)

$$\text{Jastrow} \otimes \left|\text{BCS}\right\rangle = \left[\sum_{i,j} v_{\text{PAIR}}(i,j)\,(c^{+}_{i,\uparrow} c^{+}_{j,\downarrow} + i \leftrightarrow j)\right]^{N/2}$$

WITH ~~$\uparrow\downarrow$~~

$$= \sum_{\text{VALENCE BOND}} (-1)^{\text{FERMION SIGN}} \left(\prod_{(i,j)} V_{\text{PAIR}}(i,j)\right) |\,\text{Valence Bond}\,\rangle$$

In Liang, Doucot & Anderson (PRL'88):

v_{PAIR}(i, j) = 0 if i and j connect the same sublattice
to satisfy the Marshall sign, here instead : $\bullet\!\frown\!\bullet = \frac{\uparrow\downarrow - \downarrow\uparrow}{\sqrt{2}}$

$$\boxed{\Delta_k = -\Delta_{k+Q}}$$

$|VB\rangle =$ 

It is an RVB wavefunction.!

Fermion sign $\longrightarrow$ Paring= d-wave

Why we expect superconductivity in the weakly doped t-J model ?

In absence of hole doping, consider the creator of all possible n.n. singlets :

$$\Delta^{+} = \sum_{R,\mu} \delta_{\mu}\, c^{+}_{\uparrow,R}\, c^{+}_{\uparrow,R+\tau_{\mu}}$$

by the constraint of no doubly occupied sites :

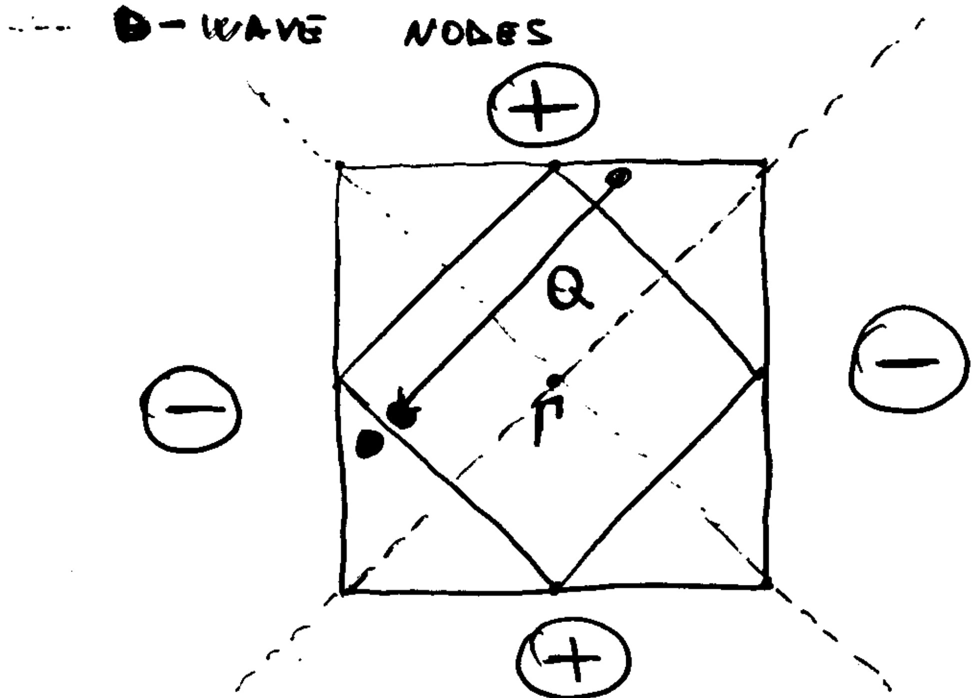
$$\Delta^{+}\Delta = -\sum_{R,\mu} (\vec{S}_{R} \vec{S}_{R+\tau_{\mu}} - \frac{n_{R} n_{R+\tau_{\mu}}}{4})$$

Thus it is a natural n.n. pairing attraction.

But why d-wave ?

From weak copuling point of view (t-J-U, Runninger '89) this maximizes the gap at the Fermi surface, yielding better kinetic energy

WEAK COUPLING ARGUMENT FOR $d_{x^2-y^2}$-WAVE



ANTIFERROMAGNETISM ⇒ PAIRING $\Delta_k = -\Delta_{k+Q}$

S-WAVE ⇒ $\Delta(k_x, k_y) = \Delta(-k_y, -k_x)$

d-WAVE ⇒ $\Delta(k_x, k_y) = - \Delta(-k_y, k_x)$

ON THE FERMI SURFACE e.g. $K_x = \pi - k_y$

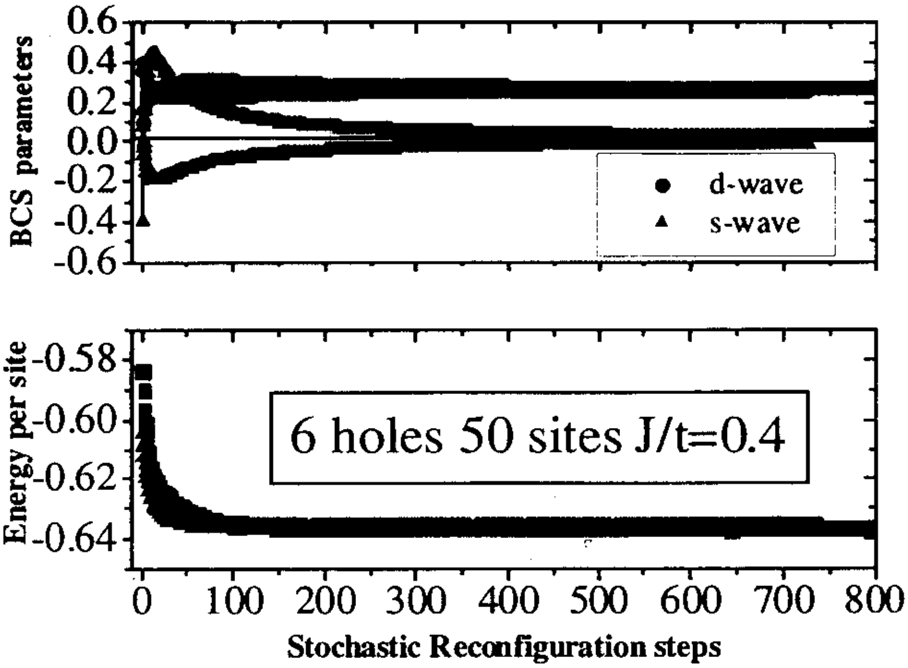
S-WAVE $\Delta_k = 0$ ALL FERMI SURFACE

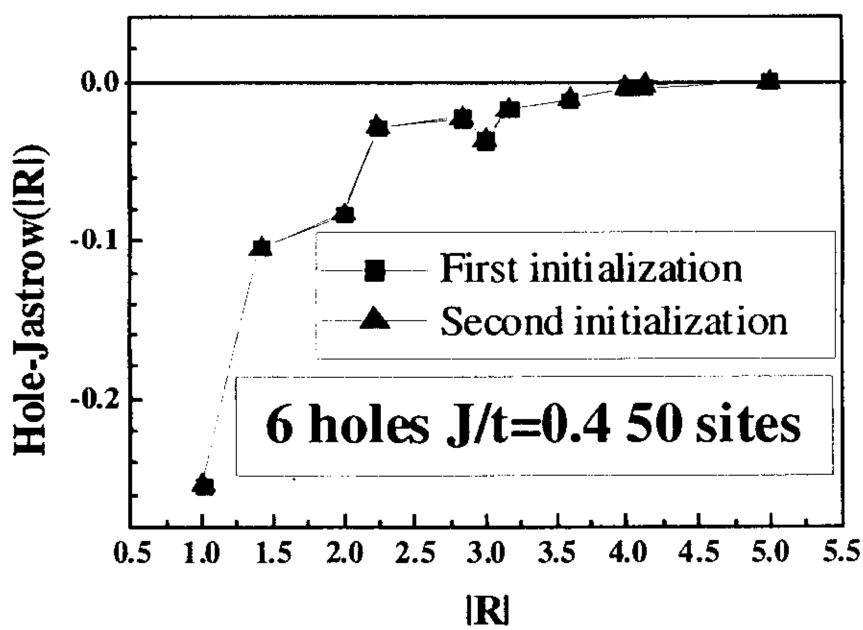
$\Delta_{d\text{-wave}} \neq 0$

⇓

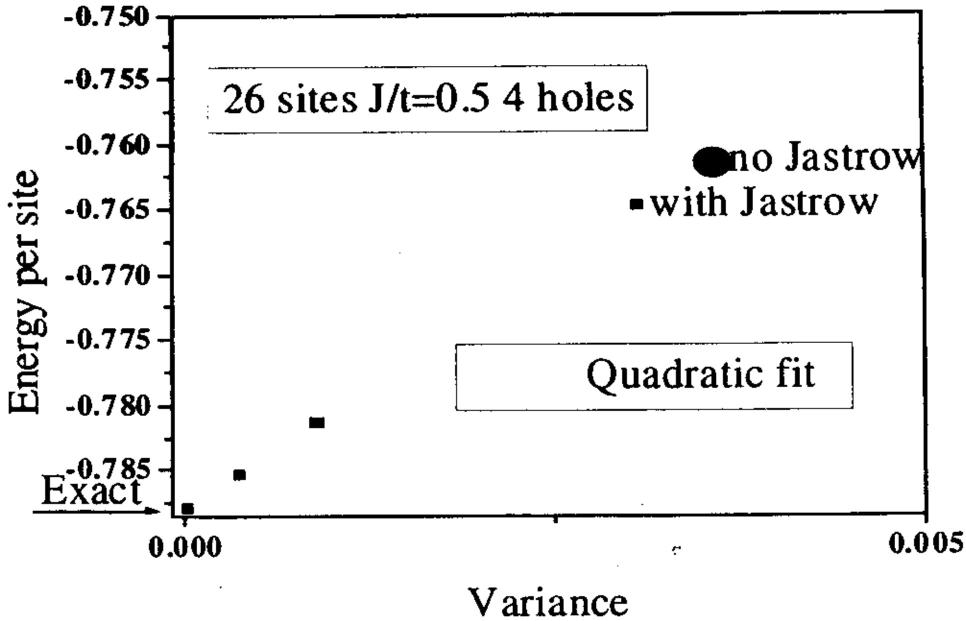
MAXIMIZES GAIN IN KINETIC ENERGY OF THE $t-J-U$ MODEL.

Starting from completely different inizializations we get the same answer

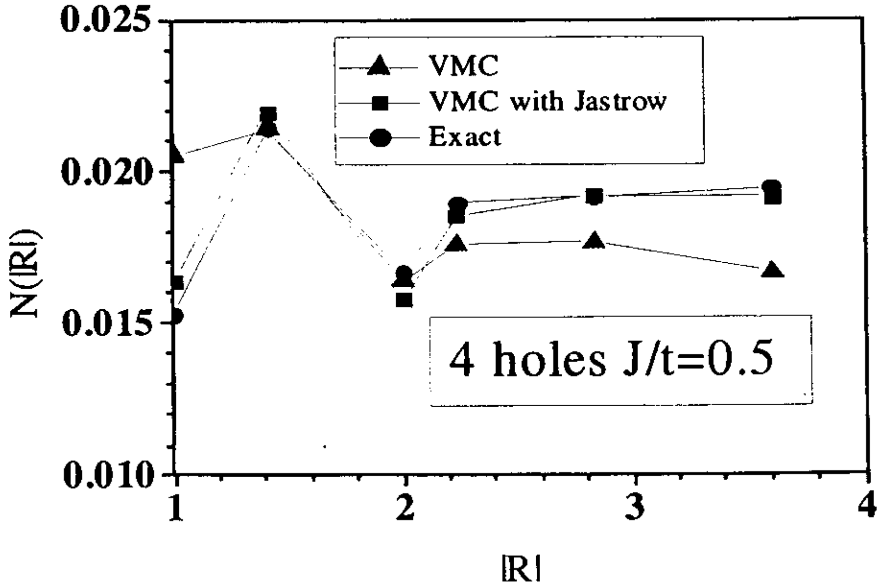




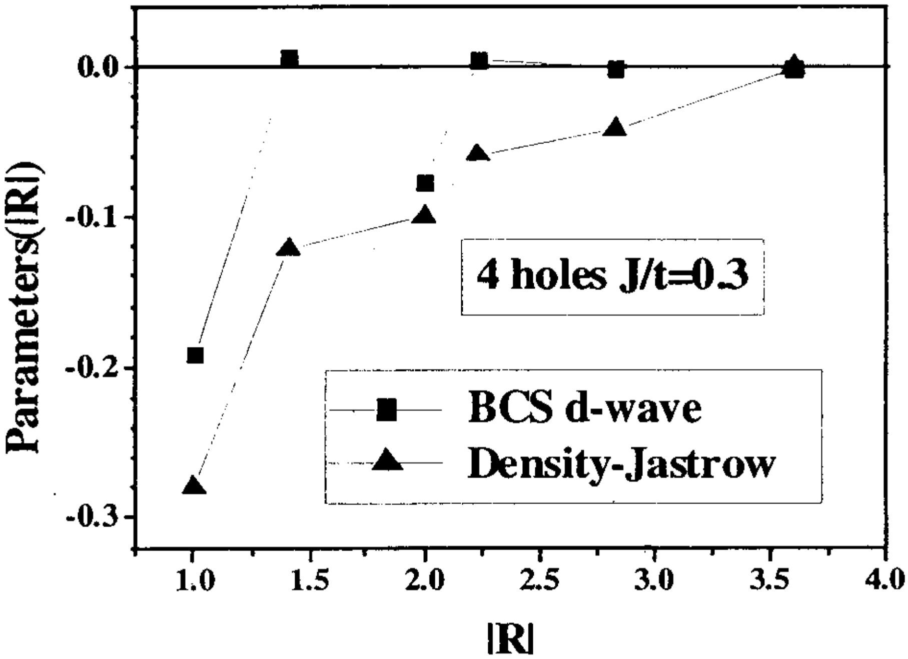
What about this wavefunction in 2D ?
doped t-J model 26 sites

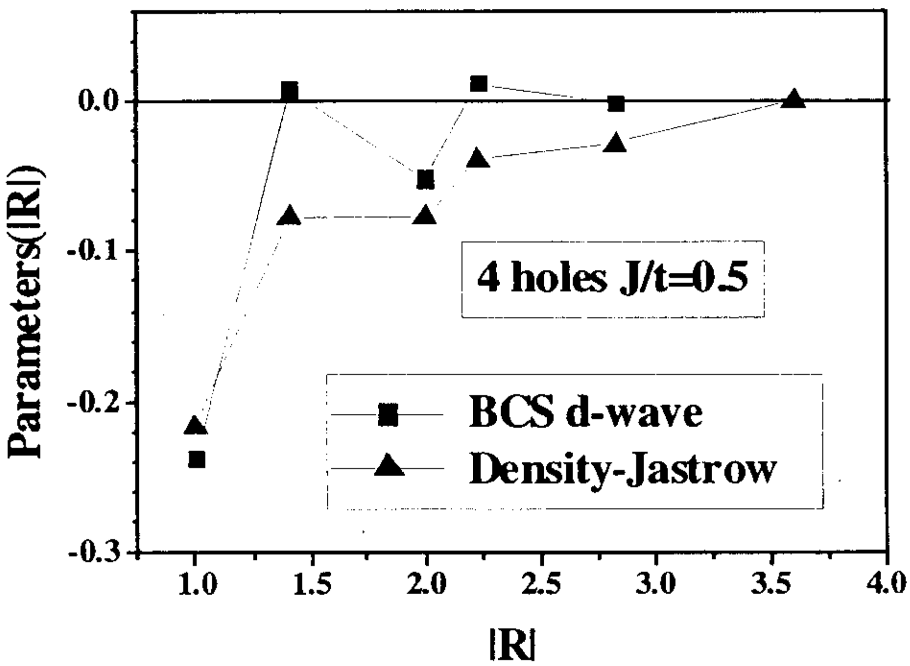


Hole-hole correlation function



Explicit pictures of the many body ground state wavefunctions

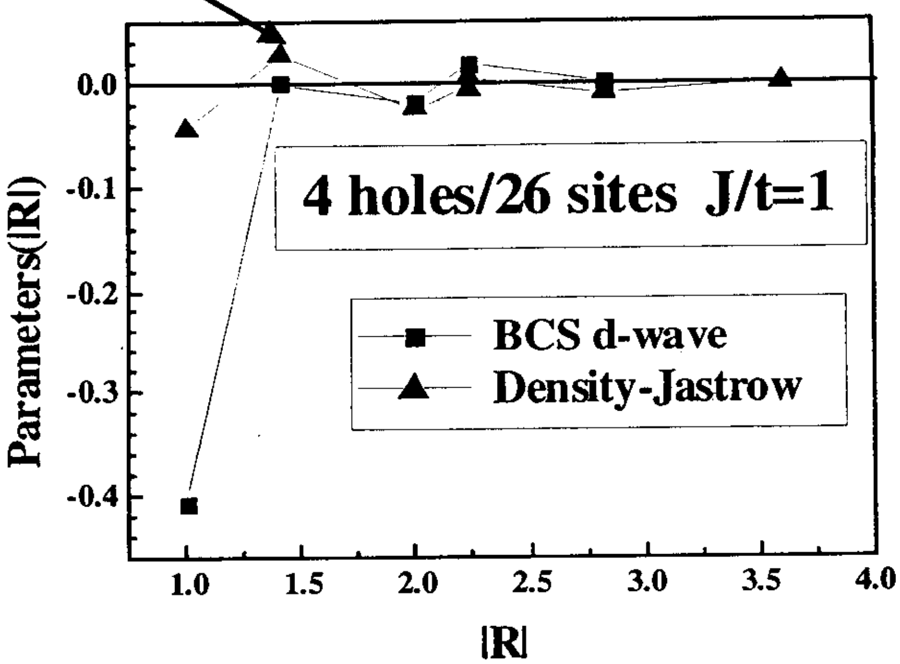


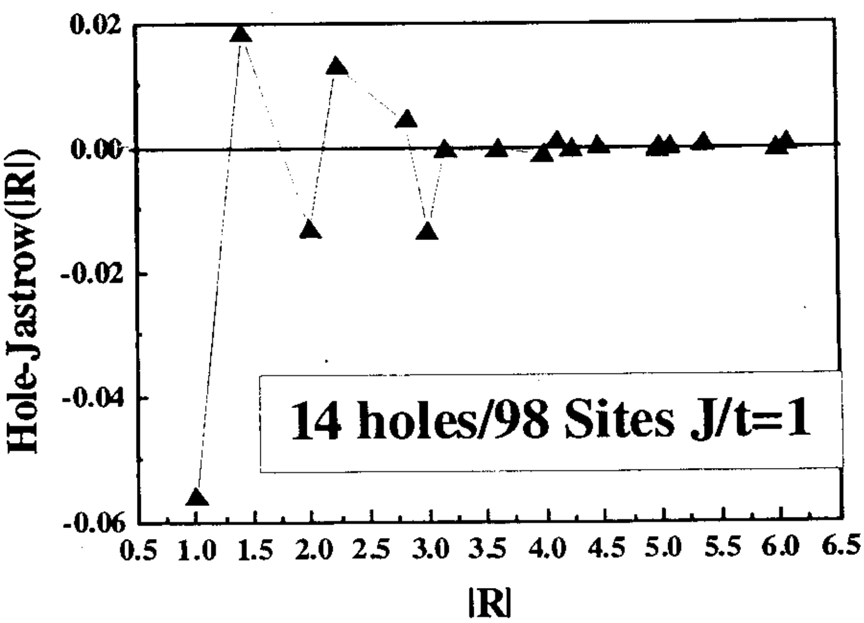


Note the strong "RVB" bond at |R|=2

Phase separation as boson condensation of d-wave BCS pairs

From repulsive to attractive n.n.n.





The structure factor N(q) diverges inside the phase separated region

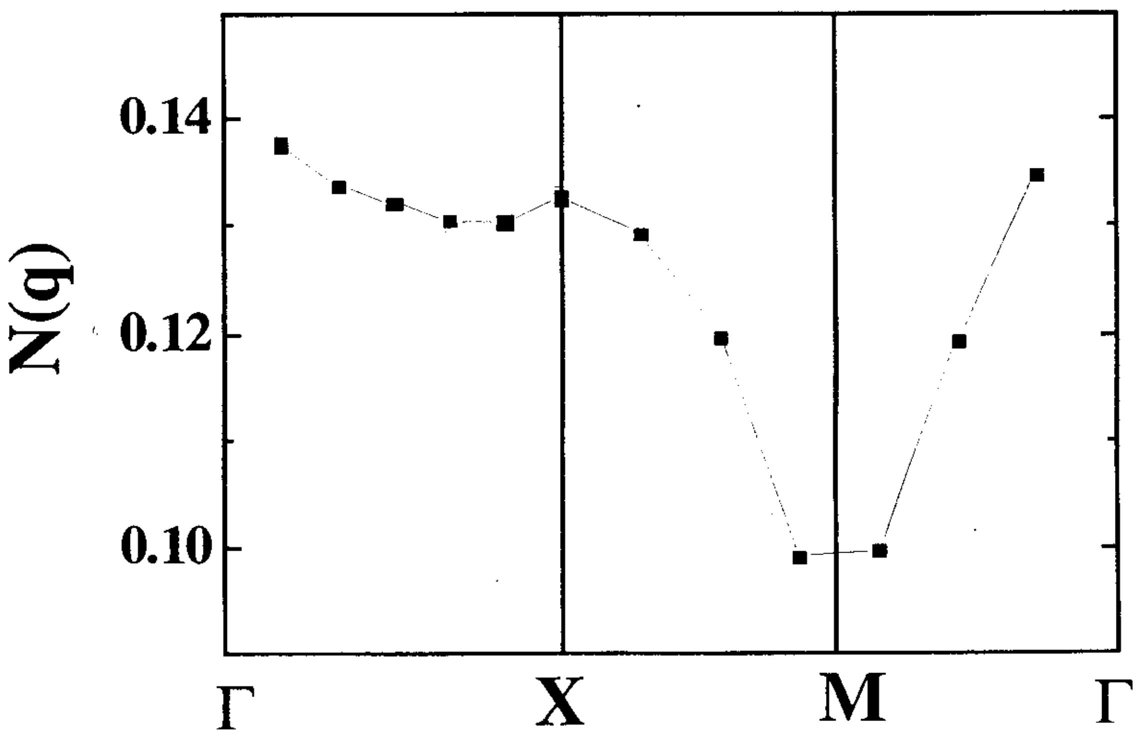
In fact from the f - sum rule:

$$\omega_q N(q) \approx q^2$$

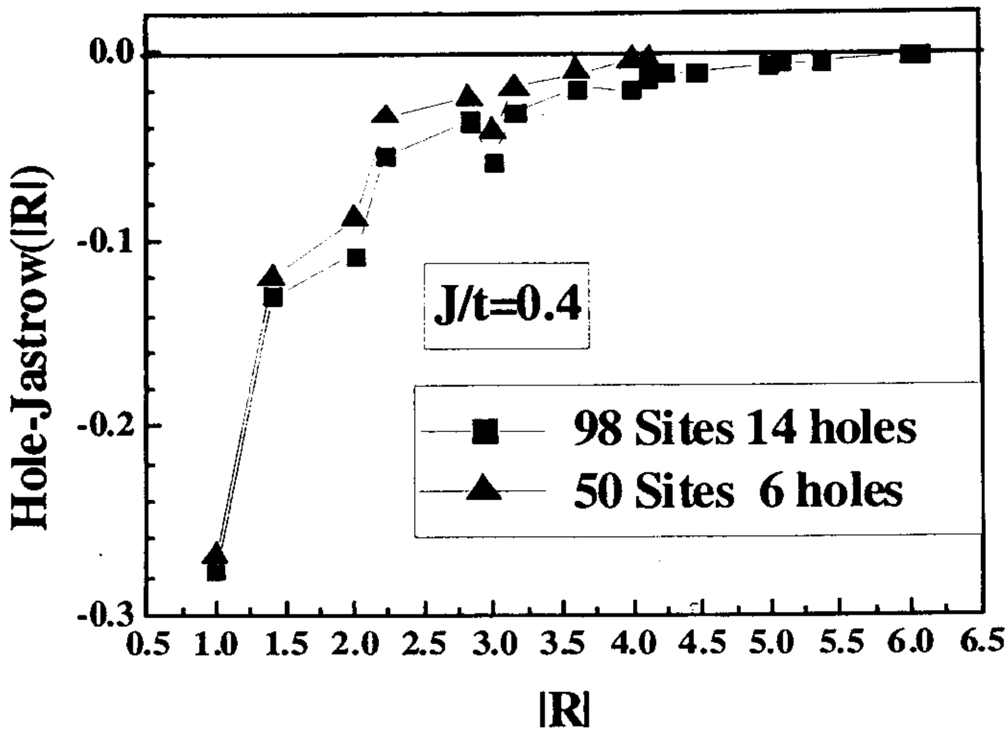
But the excitation energy $\omega_q = 0$

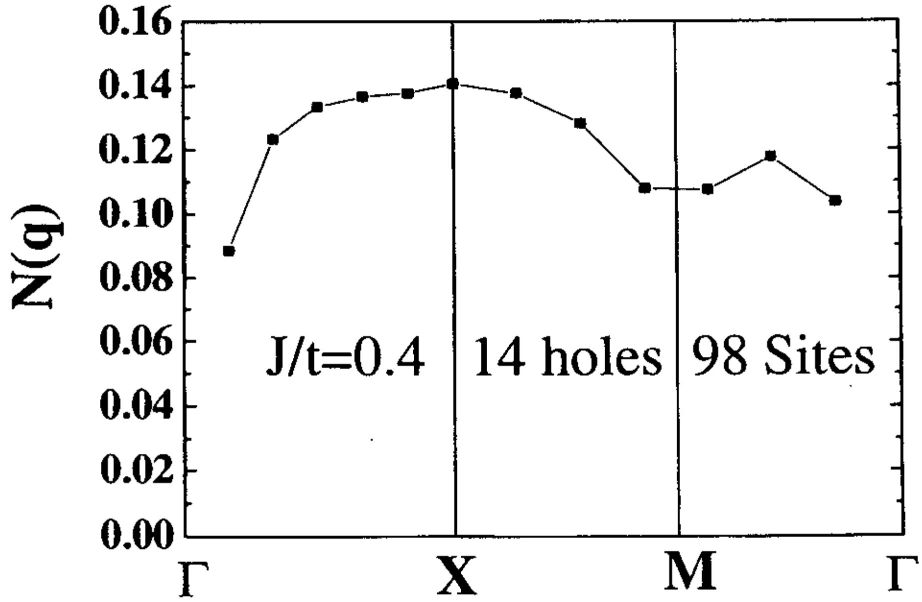
in the phase separated region $\Rightarrow N(q) \rightarrow \infty$

J/t=1 14 holes/98 Sites

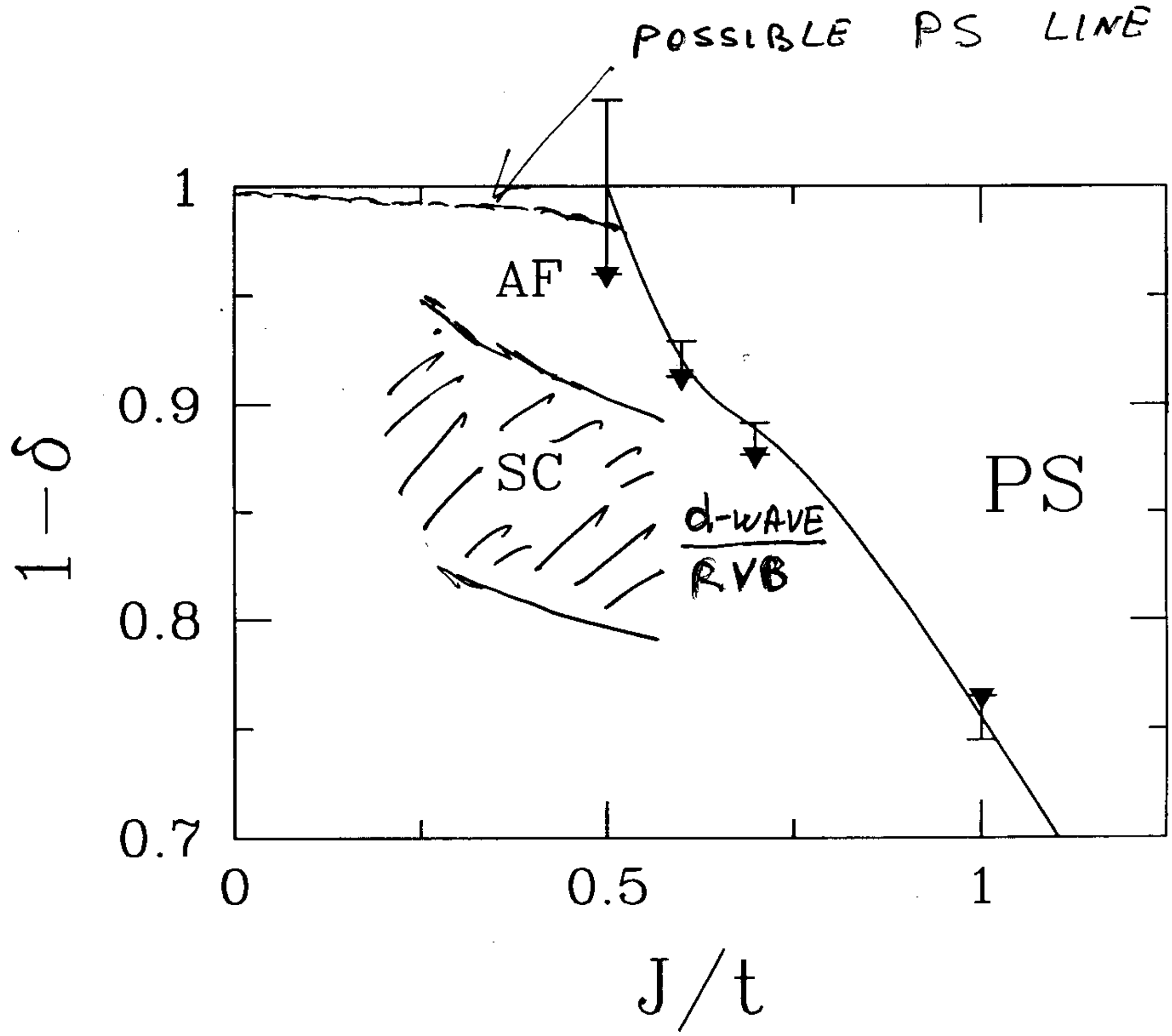


Instead in the stable d-wave phase





Phase diagram of the t-J model



M. CALANDRA & S. SORELLA PRB (2000)

Conclusions

- D-wave superconductivity from:

  J

- Importance of variational Monte Carlo to determine the ''right'' ground state .

- Two Lanczos steps over the right VMC provide ''exact'' results not only for energy.

- If nothing creazy happens as a function of system size …(stripes?)