Superconducting state of correlated metals

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Outline

1. Motivation
2. Systematic corrections to the mean field theory in the p-p and p-h channels

   Applications:
3. Superconducting phase diagram of the t-t′ Hubbard model
   d-wave region: bilayer
   p-wave region: Sr_2RuO_4
4. Van Hove density: p-p vs. p-h competition
5. Retardation effects

1. What are the distinguishing features of the superconducting state of doped Mott insulators?

pairing symmetry……………………….d-wave also at weak coupling!
particle-hole asymmetry………..?
reduced phase stiffness………..Josephson effect (RH, Hvar '02)
frequency dependence of Δ……difference w.r.t. phonons?
???

Our program

Hypothesis: supercond. in cuprates = giant Kohn-Luttinger effect

Strategy: approach from overdoped side; search for new features

Byproduct: application to Sr_2RuO_4

2. Systematic corrections to the mean field theory

Particle-particle channel
Particle-hole channel at $q=(\pi,\pi)$
Particle-hole channel at $q=0$

1. split the Hamiltonian $H = H_0 + H_1 + H_2$

$$H_1 = \frac{U}{L} \sum_{\{123\}} c^\dagger_{3\uparrow} c_{1\uparrow} c^\dagger_{4\downarrow} c_{2\downarrow} \Delta_{1234},$$

$$H_2 = \frac{U}{L} \sum_{\{123\}} c^\dagger_{3\uparrow} c_{1\uparrow} c^\dagger_{4\downarrow} c_{2\downarrow} \left(1 - \Delta_{1234}\right)$$

Kinetic energy

LARGE!

2. canonical transformation $\tilde{H} = e^{iS} H e^{-iS}$

$$S = \frac{iU}{L} \sum_{\{123\}} \frac{1 - \Delta_{1234}}{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4} c^\dagger_{3\uparrow} c_{1\uparrow} c^\dagger_{4\downarrow} c_{2\downarrow}$$

SMALL!
(can be treated
by mean field)

3. resulting Hamiltonian $\tilde{H} = H_0 + H_1 + \tilde{H}_2$

where

$$\tilde{H}_2 = -\frac{U^2}{2L^2} \sum_{\{123\}} \sum_{\{\alpha\beta\gamma\}} \frac{(1 - \Delta_{1234})(1 + \Delta_{\alpha\beta\gamma\delta})}{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4} \times \Big[(\delta_{1\gamma} c^\dagger_{3\uparrow} c_{\alpha\uparrow} - \delta_{3\alpha} c^\dagger_{\gamma\uparrow} c_{1\uparrow}) c^\dagger_{4\downarrow} c_{2\downarrow} c^\dagger_{\delta\downarrow} c_{\beta\downarrow} + (\delta_{2\delta} c^\dagger_{4\downarrow} c_{\beta\downarrow} - \delta_{4\beta} c^\dagger_{\delta\downarrow} c_{2\downarrow}) c^\dagger_{\gamma\uparrow} c_{\alpha\uparrow} c^\dagger_{3\uparrow} c_{1\uparrow} \Big].$$

BCS channel

$$\Delta_{1234} = 1 \ \text{for} \ \mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4 = 0,$$

$$\Delta_{1234} = 0 \ \text{otherwise.}$$

Density wave channel

$$\Delta_{1234} = 1 \ \text{for} \ \mathbf{k}_3 - \mathbf{k}_1 = \mathbf{Q} \ \text{or} \ \mathbf{k}_3 - \mathbf{k}_2 = \mathbf{Q}$$

$$\Delta_{1234} = 0 \ \text{otherwise.}$$

Landau channel

$$\Delta_{1234} = 1 \ \text{for} \ \mathbf{k}_3 = \mathbf{k}_1 \ \text{or} \ \mathbf{k}_3 = \mathbf{k}_2$$

$$\Delta_{1234} = 0 \ \text{otherwise.}$$

Kohn-Luttinger superconductivity: variational approach

variational wave function: $|\psi\rangle = e^{-iS}\prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow})|0\rangle = e^{-iS}|\tilde{\psi}\rangle$

expectation value of the energy in the state $|\psi\rangle$:

$$E = \langle\tilde{\psi}|\tilde{H}|\tilde{\psi}\rangle = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} f_{\mathbf{k}\sigma} + \frac{U^2}{L^2}\sum\nolimits'_{\{\mathbf{k}\}} \frac{f_1 f_2 (1-f_3)(1-f_4)}{\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4} + \frac{1}{L}\sum_{\mathbf{kp}} V_{\mathbf{kp}} b^*_{\mathbf{k}} b_{\mathbf{p}} + \mathrm{const}$$

order parameter $b_{\mathbf{p}} = \langle\tilde{\psi}|c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow}|\tilde{\psi}\rangle$

effective interaction $V_{\mathbf{kp}} = U + U^2 \mathrm{Re}\chi(\mathbf{k}+\mathbf{p}, \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}})$

susceptibility $\chi(\mathbf{q},\omega) = \frac{1}{L}\sum_{\mathbf{K}} \frac{f_{\mathbf{K}} - f_{\mathbf{K}+\mathbf{q}}}{\varepsilon_{\mathbf{K}+\mathbf{q}} - \varepsilon_{\mathbf{K}} - \omega - i0}$

gap equation $\boxed{\Delta_{\mathbf{k}} = -\frac{1}{L}\sum_{\mathbf{p}} V_{\mathbf{kp}} \Delta_{\mathbf{p}} \frac{\tanh(E_{\mathbf{p}}/2T)}{2E_{\mathbf{p}}}}$

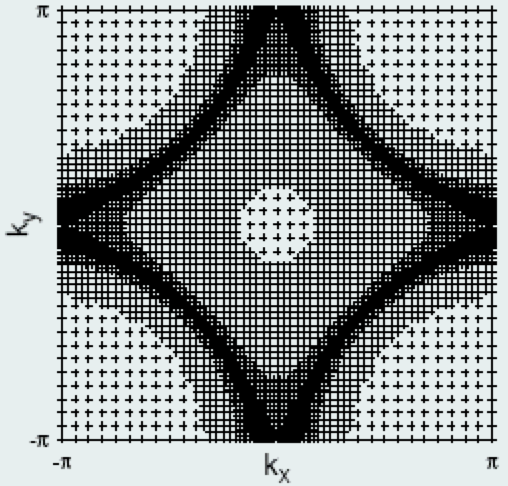
quasiparticle energy $E_{\mathbf{p}} = (\varepsilon^2_{\mathbf{p}} + \Delta^2_{\mathbf{p}})^{1/2}$

Numerical techniques for $\boxed{\Delta_{\mathbf{k}} = -\frac{1}{L}\sum_{\mathbf{p}} V_{\mathbf{kp}}\Delta_{\mathbf{p}}\frac{\tanh(E_{\mathbf{p}}/2T)}{2E_{\mathbf{p}}}}$

FFT:

$$\chi(\mathbf{q},\omega) = \frac{1}{L}\sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k+q}}}{\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k}} - \omega - i0}$$

Lattice:



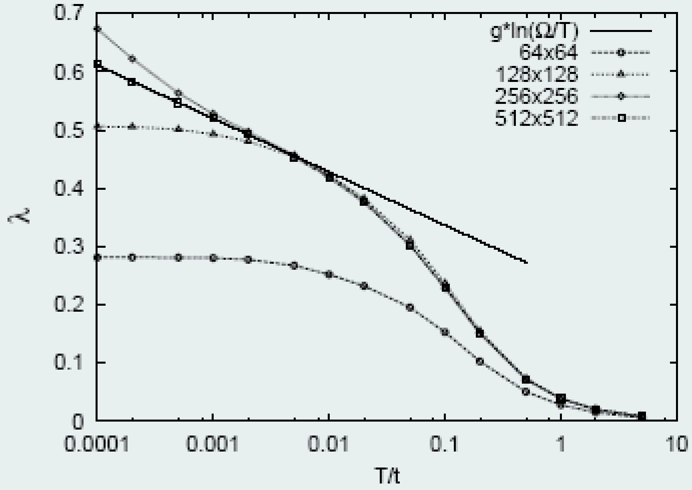
$t'/t = 0.3$ a $\rho = 0.8$.

Lanczos diagonalization: calculation of T_c

Linearized gap equation:

$D_{\mathbf{k}} = \sum_{\mathbf{p}} I_{\mathbf{kp}}(T) D_{\mathbf{p}}$ where $D_{\mathbf{k}} \propto \Delta_{\mathbf{k}}$

condition: $\lambda(T_c) = 1$



d_{xy} sector, $U = W/2$, $t'/t = 0.78$ a $\rho = 1$.

Symmetry: 5 irreducibile representations

Iterative solution: for $T < T_c$; brute force

Density wave channel

Order parameters

$$d^0_{\mathbf{k}} = \frac{1}{2}\sum_{\sigma}\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle,$$

$$\vec{d}_{\mathbf{k}} = \frac{1}{2}\sum_{\alpha\beta}\langle c^\dagger_{\mathbf{k}\alpha}\vec{\sigma}_{\alpha\beta} c_{\mathbf{k}\beta}\rangle$$

Variational energy

$$\boxed{E = \sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}} f_{\mathbf{k}\sigma} - \frac{1}{L}\sum_{\mathbf{k},\mathbf{p}}\left[V^{\mathrm{cdw}}_{\mathbf{kp}} d^0_{\mathbf{k}} d^0_{\mathbf{p}} + V^{\mathrm{sdw}}_{\mathbf{kp}}\vec{d}_{\mathbf{k}}\cdot\vec{d}_{\mathbf{p}}\right]}$$

where

$$V^{\mathrm{sdw}}_{\mathbf{kp}} = U - \frac{U^2}{2}\left[\chi'_{\mathrm{pp}}(\mathbf{k}+\mathbf{p},\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{p}}) + \chi'_{\mathrm{pp}}(\mathbf{k}+\mathbf{p},\varepsilon_{\bar{\mathbf{k}}}+\varepsilon_{\bar{\mathbf{p}}})\right]$$

$$\begin{aligned} V^{\mathrm{cdw}}_{\mathbf{kp}} &= -U + \frac{U^2}{2}\left[\chi'_{\mathrm{pp}}(\mathbf{k}+\mathbf{p},\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{p}}) + \chi'_{\mathrm{pp}}(\mathbf{k}+\mathbf{p},\varepsilon_{\bar{\mathbf{k}}}+\varepsilon_{\bar{\mathbf{p}}})\right] \\ &\quad -U^2\left[\chi'_{\mathrm{ph}}(\mathbf{k}-\bar{\mathbf{p}},\varepsilon_{\mathbf{k}}-\varepsilon_{\bar{\mathbf{p}}}) + \chi'_{\mathrm{ph}}(\bar{\mathbf{k}}-\mathbf{p},\varepsilon_{\bar{\mathbf{k}}}-\varepsilon_{\mathbf{p}})\right], \end{aligned}$$

particle-particle susc.

$$\chi_{\mathrm{pp}}(\mathbf{q},\omega) = \frac{1}{L}\sum_{\mathbf{K}}\frac{1-f_{\mathbf{K}}-f_{\mathbf{q}-\mathbf{K}}}{\varepsilon_{\mathbf{K}}+\varepsilon_{\mathbf{q}-\mathbf{K}}-\omega-i0}$$

Gap functions

$$\Delta^0_{\mathbf{k}} = \frac{1}{L}\sum_{\mathbf{p}} V^{\mathrm{cdw}}_{\mathbf{kp}} d^0_{\mathbf{p}},$$

$$\vec{\Delta}_{\mathbf{k}} = \frac{1}{L}\sum_{\mathbf{p}} V^{\mathrm{sdw}}_{\mathbf{kp}} \vec{d}_{\mathbf{p}}.$$

SDW case: $H = \sum_{\mathbf{k}}{}' (\hat{c}_{\mathbf{k}})^\dagger N_{\mathbf{k}} \hat{c}_{\mathbf{k}} + \sum_{\mathbf{k}} \vec{d}_{\mathbf{k}} \cdot \vec{\Delta}_{\mathbf{k}}$

4-vector $(\hat{c}_{\mathbf{k}})^\dagger = (c^\dagger_{\mathbf{k}\uparrow}, c^\dagger_{\mathbf{k}\downarrow}, c^\dagger_{\bar{\mathbf{k}}\uparrow}, c^\dagger_{\bar{\mathbf{k}}\downarrow})$ $\delta_{\mathbf{k}} = (\varepsilon_{\mathbf{k}} - \varepsilon_{\bar{\mathbf{k}}})/2,\ \omega_{\mathbf{k}} = (\varepsilon_{\mathbf{k}} + \varepsilon_{\bar{\mathbf{k}}})/2$

4x4 matrix $N_{\mathbf{k}} = \omega_{\mathbf{k}} + \begin{pmatrix} \delta_{\mathbf{k}} & -\vec{\Delta}^*_{\mathbf{k}} \cdot \vec{\sigma} \\ -\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma} & -\delta_{\mathbf{k}} \end{pmatrix}$ $\vec{Q}_{\mathbf{k}} = \vec{\Delta}_{\mathbf{k}} \times \vec{\Delta}^*_{\mathbf{k}}$

unitary state: $\vec{Q}_{\mathbf{k}} = 0$

eigenvalues $E_{\mathbf{k}} = \sqrt{\delta^2_{\mathbf{k}} + |\vec{\Delta}_{\mathbf{k}}|^2 \pm |\vec{Q}_{\mathbf{k}}|^2}$

gap equation:
(unitary states)

$$\vec{\Delta}_{\mathbf{k}} = \frac{1}{L}\sum_{\mathbf{p}} V^{\mathrm{sdw}}_{\mathbf{kp}} \vec{\Delta}^*_{\mathbf{p}} \frac{f_{\mathbf{p}2} - f_{\mathbf{p}1}}{E_{\mathbf{p}1} - E_{\mathbf{p}2}}$$

Classification of symmetry breaking solutions

Channel: BCS, density wave, Landau

Spin sector: singlet,triplet

Orbital sector (2D square lattice): s, d, d_{xy}, g, p

Charge density wave channel: $\Delta^0_{\mathbf{k}} = x_{\mathbf{k}} + i y_{\mathbf{k}}$ $\quad x_{\bar{\mathbf{k}}} = x_{\mathbf{k}}$ and $y_{\bar{\mathbf{k}}} = -y_{\mathbf{k}}$

$$\begin{pmatrix} x_{\mathbf{k}} \\ y_{\mathbf{k}} \end{pmatrix} = \frac{1}{L} \sum_{\mathbf{p}} V^{\mathrm{cdw}}_{\mathbf{kp}} \begin{pmatrix} x_{\mathbf{p}} \\ -y_{\mathbf{p}} \end{pmatrix} \frac{f_{\mathbf{p}2} - f_{\mathbf{p}1}}{E_{\mathbf{p}1} - E_{\mathbf{p}2}}$$

(Hankevych,Wegner, EPJ ’03)

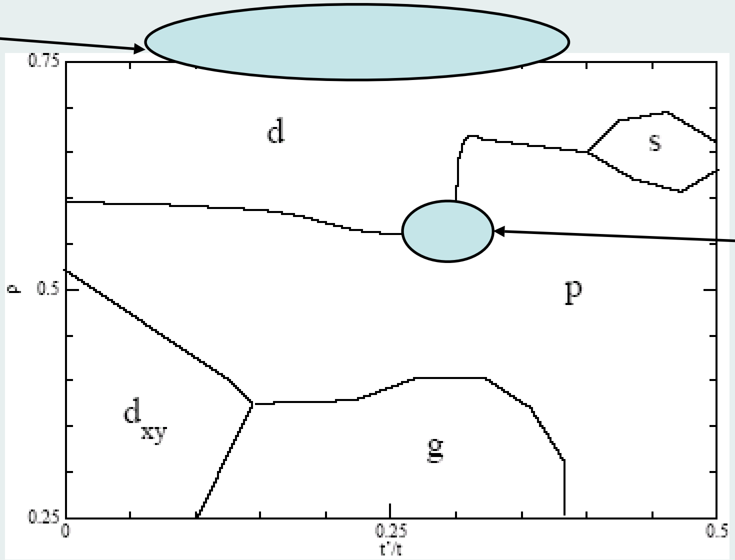
Spin density wave channel: $\vec{\Delta}_{\mathbf{k}} = (x_{\mathbf{k}} + i y_{\mathbf{k}})\vec{n}$ (“axial” states)

$$\begin{pmatrix} x_{\mathbf{k}} \\ y_{\mathbf{k}} \end{pmatrix} = \frac{1}{L} \sum_{\mathbf{p}} V^{\mathrm{sdw}}_{\mathbf{kp}} \begin{pmatrix} x_{\mathbf{p}} \\ -y_{\mathbf{p}} \end{pmatrix} \frac{f_{\mathbf{p}2} - f_{\mathbf{p}1}}{E_{\mathbf{p}1} - E_{\mathbf{p}2}}$$

3. Superconducting phase diagram of the t-t' Hubbard model

Superconducting phase diagram of the Hubbard model in the plane ρ vs. t'/t

(U infinitesimal)



cuprates

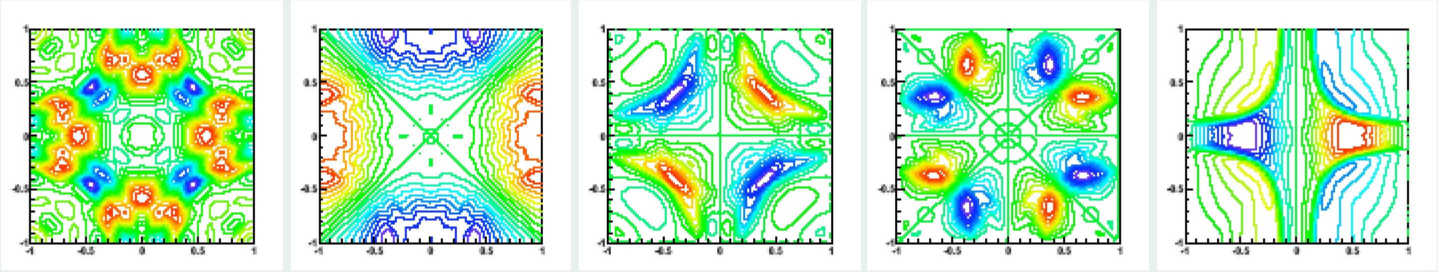
ρ

Sr_2RuO_4

t'/t

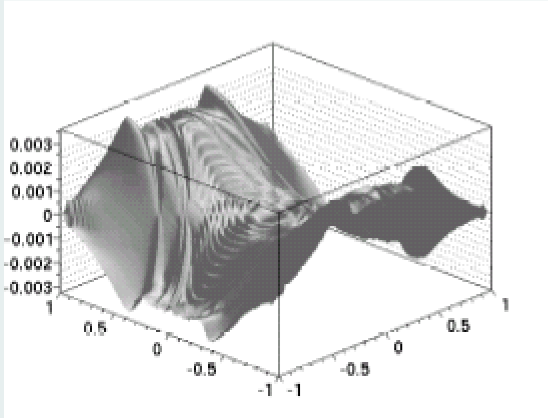
R.H., Phys. Rev. B **59**, 9600 (1999)

Pairing symmetries:

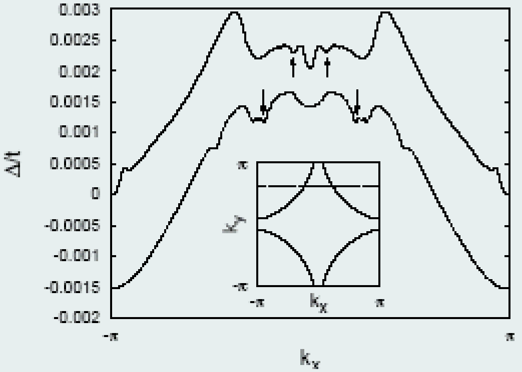


s d d_{xy} g p

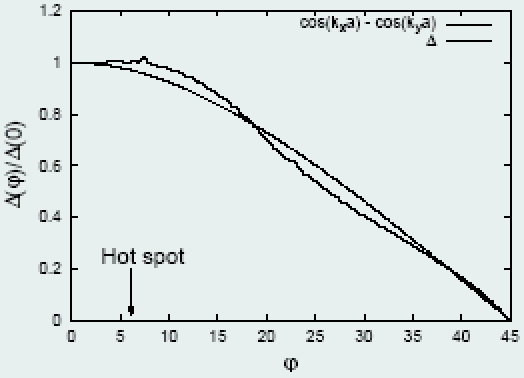
d-wave region: cuprates $t'/t = 0.3$, $\rho = 0.8$, $U/t = 4 \Rightarrow T_c = 0.0013t$



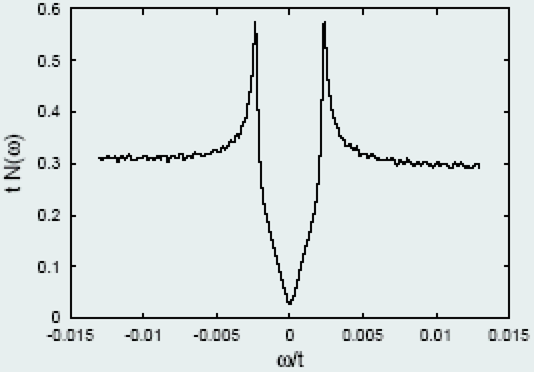
$\Delta_{\mathbf{k}}$ in the 1^{st} BZ.



$\Delta_{\mathbf{k}}$ along $k_y = \pi$ and $k_y = 5\pi/8$.



$\Delta_{\mathbf{k}}$ along the Fermi line.



DOS : $N(\omega) = L^{-1} \sum_{\mathbf{k}} [u_{\mathbf{k}}^2 \delta(\omega - E_{\mathbf{k}}) + v_{\mathbf{k}}^2 \delta(\omega + E_{\mathbf{k}})]$

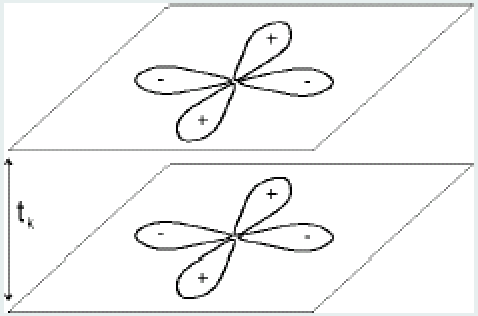
Hubbard model on a bilayer

Maximal transition temperatures for various families of cuprate superconductors:

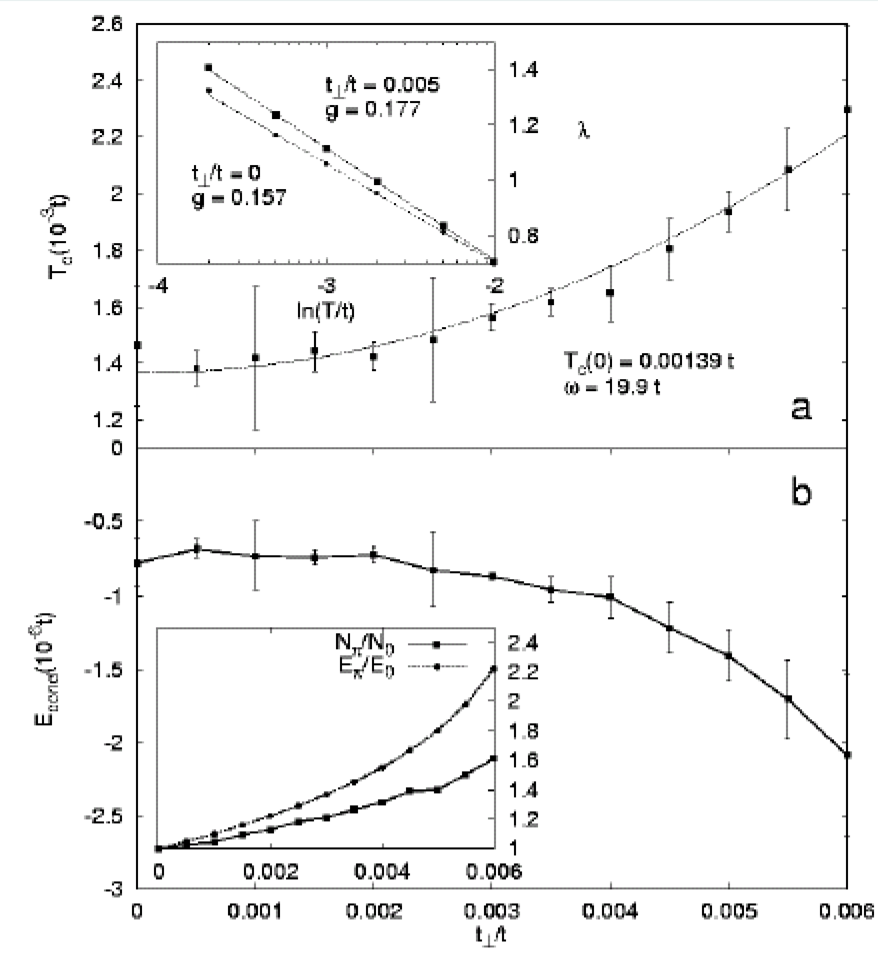
	$n=1$	$n=2$	$n=3$
$Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$	38	92	110
$TlBa_2Ca_{n-1}Cu_nO_{2n+3}$	9	80	120
$Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$	90	110	125
$HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$	95	114	133

Interplane hopping:
$t_{\mathbf{k}} = 4t_\perp(\cos k_x - \cos k_y)^2$
bonding band: $k_z = 0$, $\varepsilon_{\mathbf{k}} - t_{\mathbf{k}}$
antibonding band: $k_z = \pi$, $\varepsilon_{\mathbf{k}} + t_{\mathbf{k}}$
gap equation (α, β=bonding, antibonding)

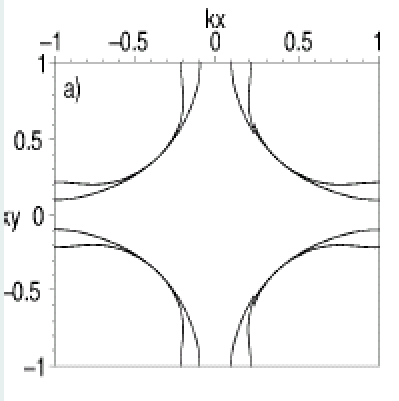
$$\boxed{\Delta^\alpha_{\mathbf{k}} = -\frac{1}{L}\sum_{\mathbf{p}\beta} V^{\alpha\beta}_{\mathbf{kp}}\Delta^\beta_{\mathbf{p}}\frac{\tanh(E^\beta_{\mathbf{p}}/2T)}{2E^\beta_{\mathbf{p}}}}$$



Hubbard model on a bilayer



transition temperature
$T_c \propto e^{-1/g}$

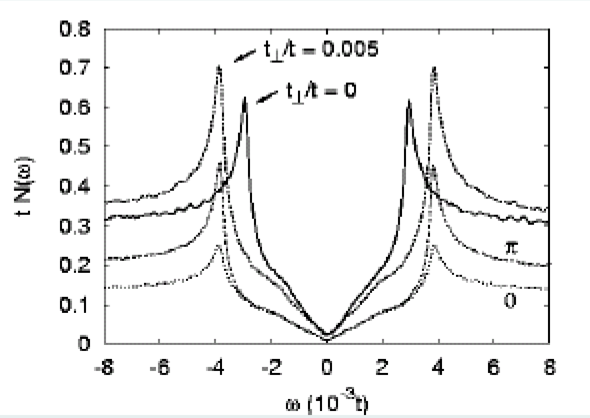


enhanced DOS at the Van Hove point implies $\delta g > 0$

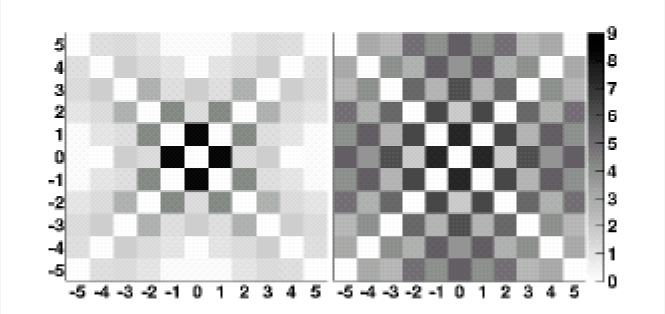
$$\frac{\delta T_c}{T_c} \approx \frac{\delta g}{g^2}$$

δT_c can be large
even for $\delta g / g \ll 1$

Hubbard model on a bilayer

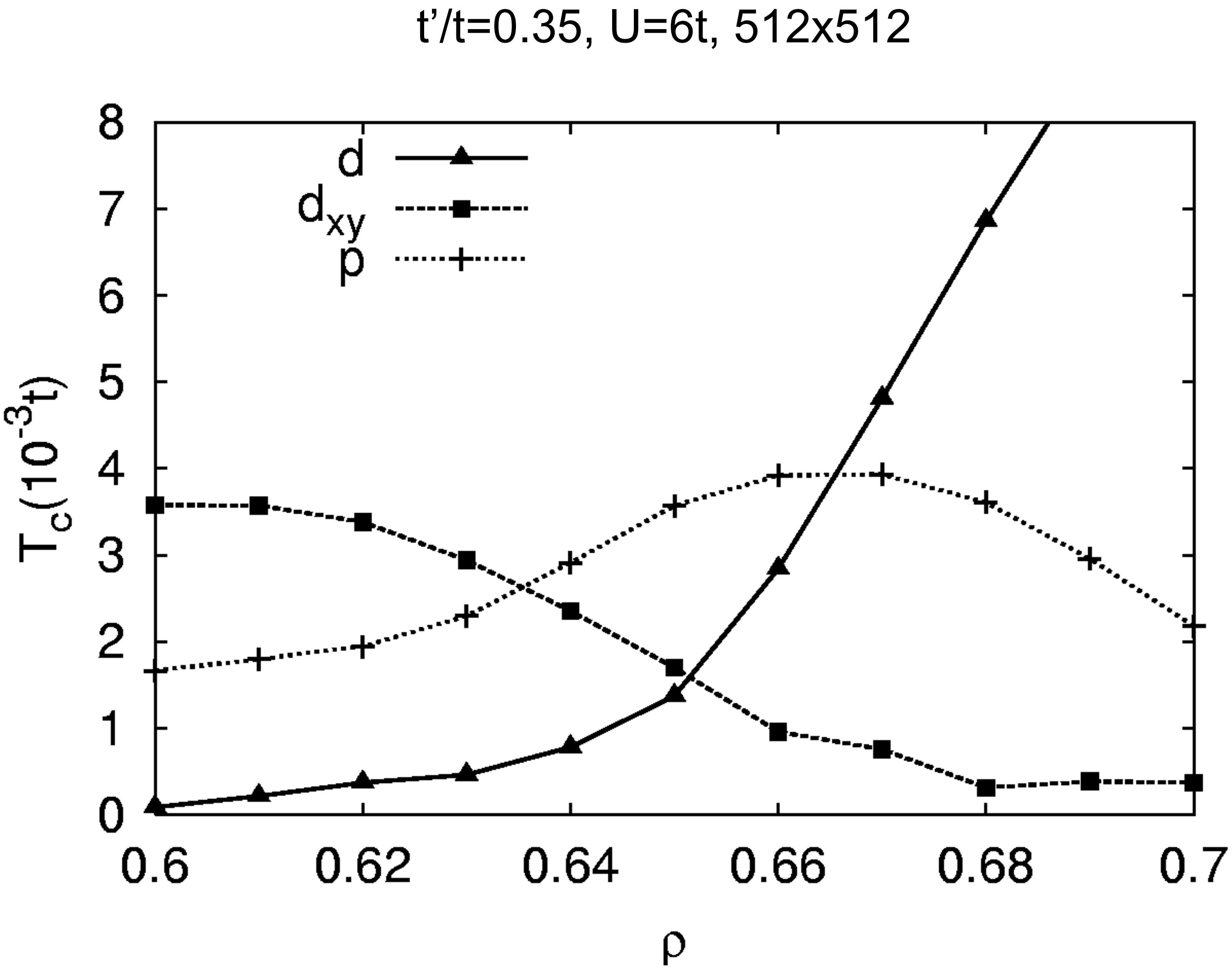


both Δ^0 and Δ^π grow w. r. t. single plane,
but $\Delta^0 - \Delta^\pi$ remains small
(in agreement with ARPES)

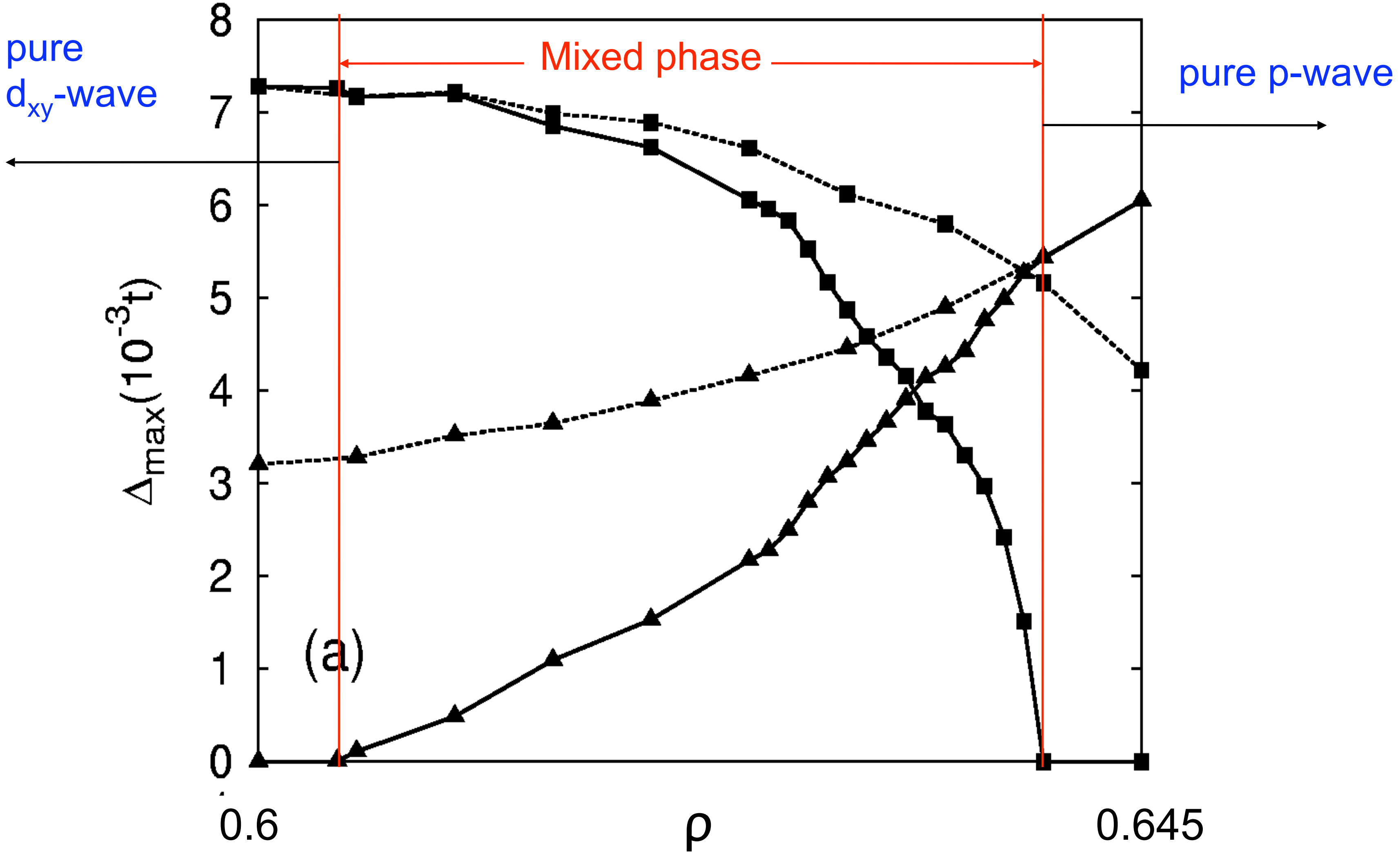


Pairing functions $F_{ij}^{\alpha\beta} = \sum_\sigma \sigma \langle c_{i-\sigma}^{\alpha} c_{j\sigma}^{\beta} \rangle$
Left panel: in-plane pairing function
$F_{ij}^{\parallel} = \left(F_{ij}^{00} + F_{ij}^{\pi\pi} \right) /2$
Right panel: interplane pairing function
$F_{ij}^{\perp} = \left(F_{ij}^{00} - F_{ij}^{\pi\pi} \right) /2$

Transition temperatures for singlet and triplet pairing



Triplet-singlet mixing



Mixed phase - correlation functions

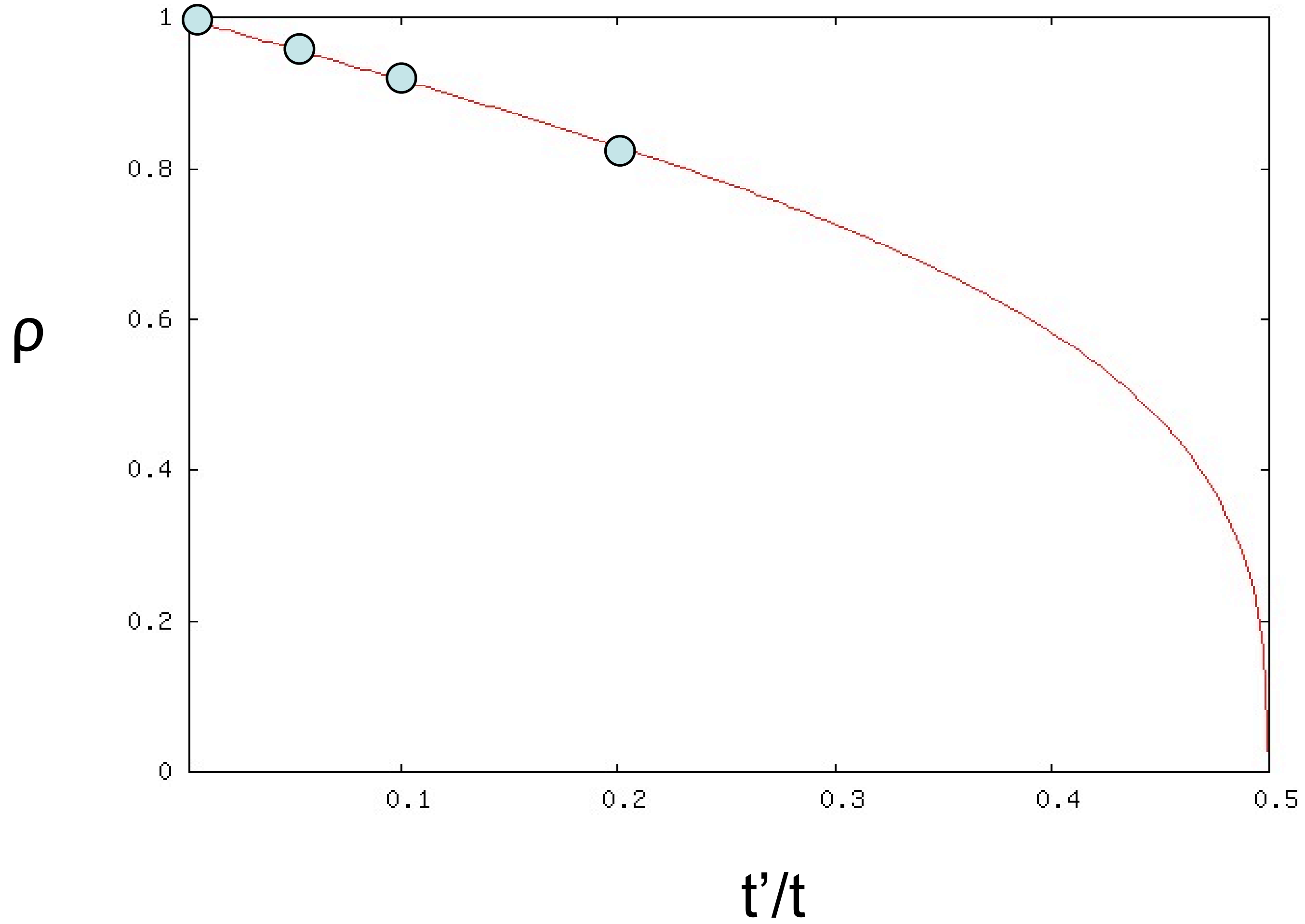
a unitary triplet-singlet mixture is possible only if the triplet state is planar

symmetry properties in the planar, axial, and mixed planar phases:

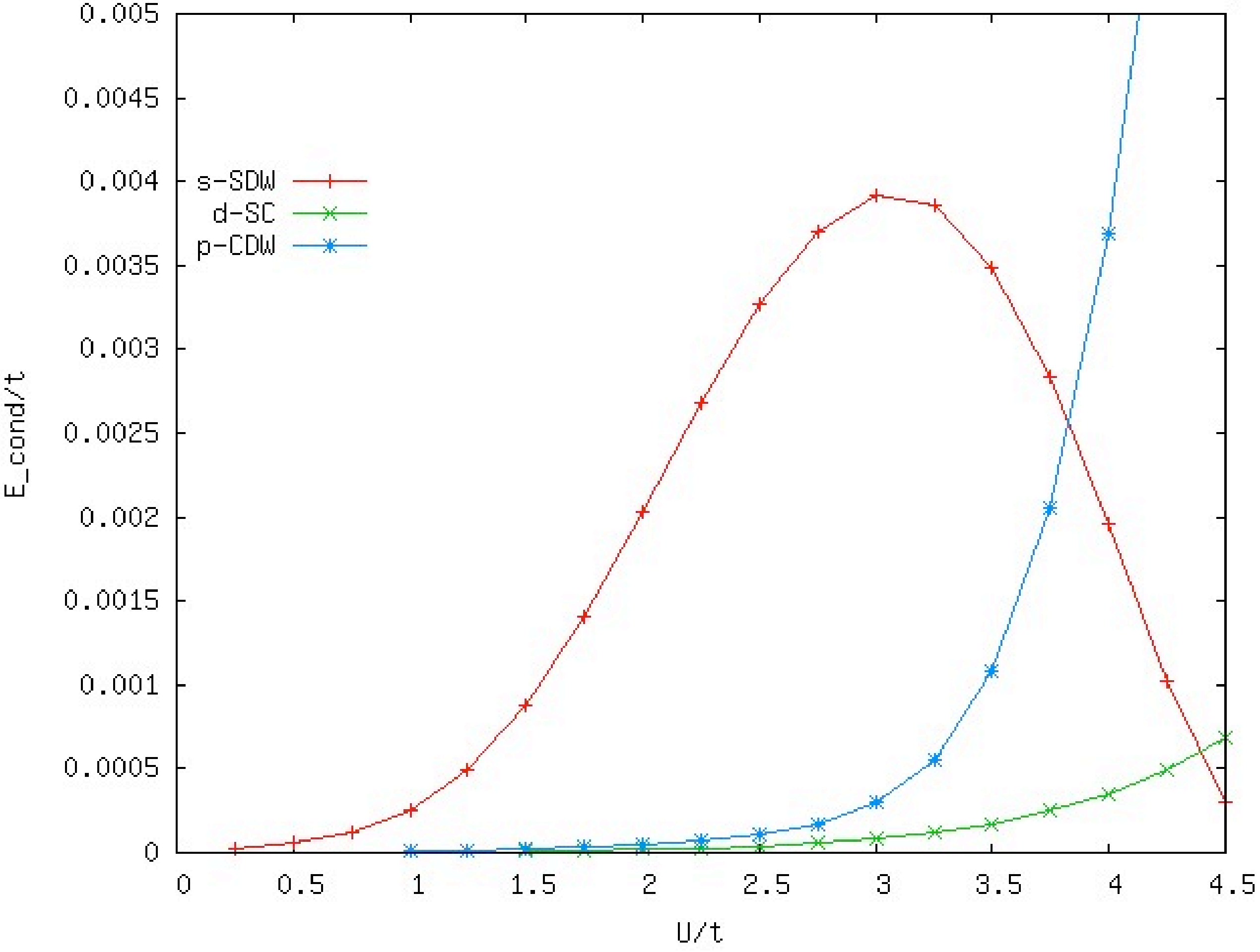
	Planar	Axial	Mixed planar
T	yes	broken	broken
P	yes	yes	broken
TP	yes	broken	yes
$\mathbf{C}_{ij}$	0	0	finite
B_{ijk}	0	finite	0

the density-spin correlation, $\mathbf{C}_{ij} = \langle n_i \mathbf{S}_j \rangle$
density-current correlation, $B_{ijk} = \langle n_i j_{jk} \rangle$

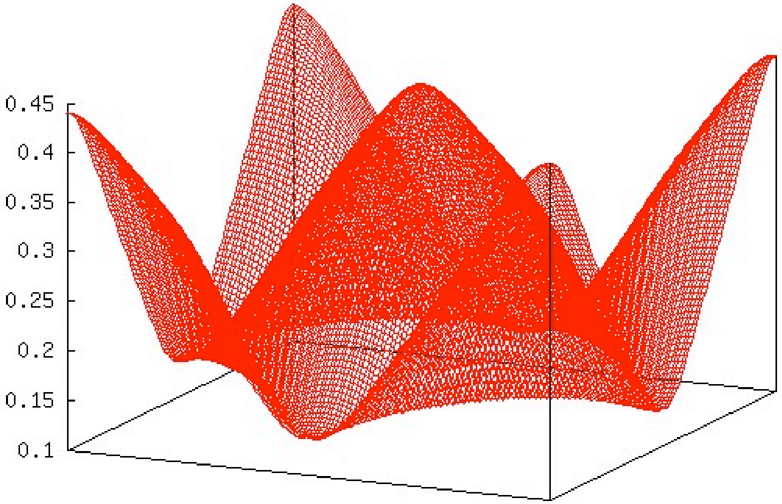
4. Competition between particle-particle and particle-hole instabilities at the Van Hove density



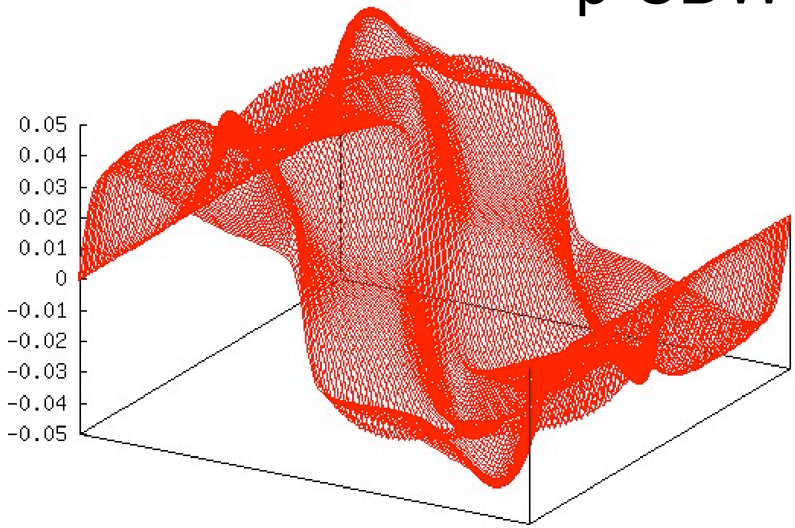
t'/t=0.0, Van Hove density, 128x128



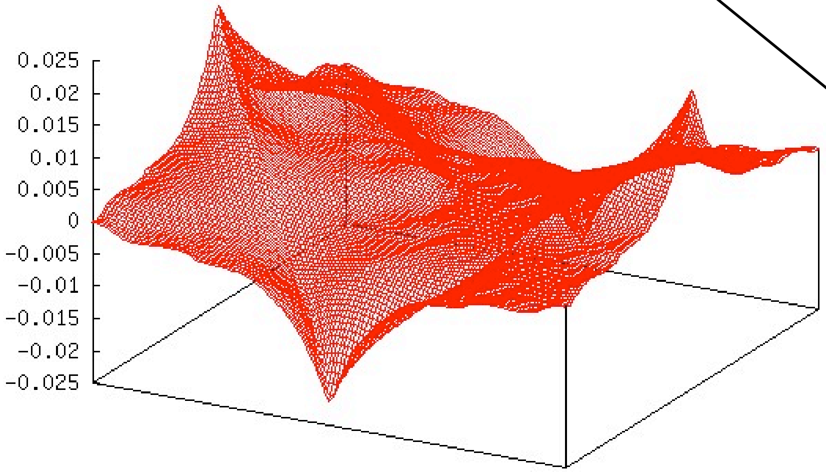
s-SDW



p-CDW



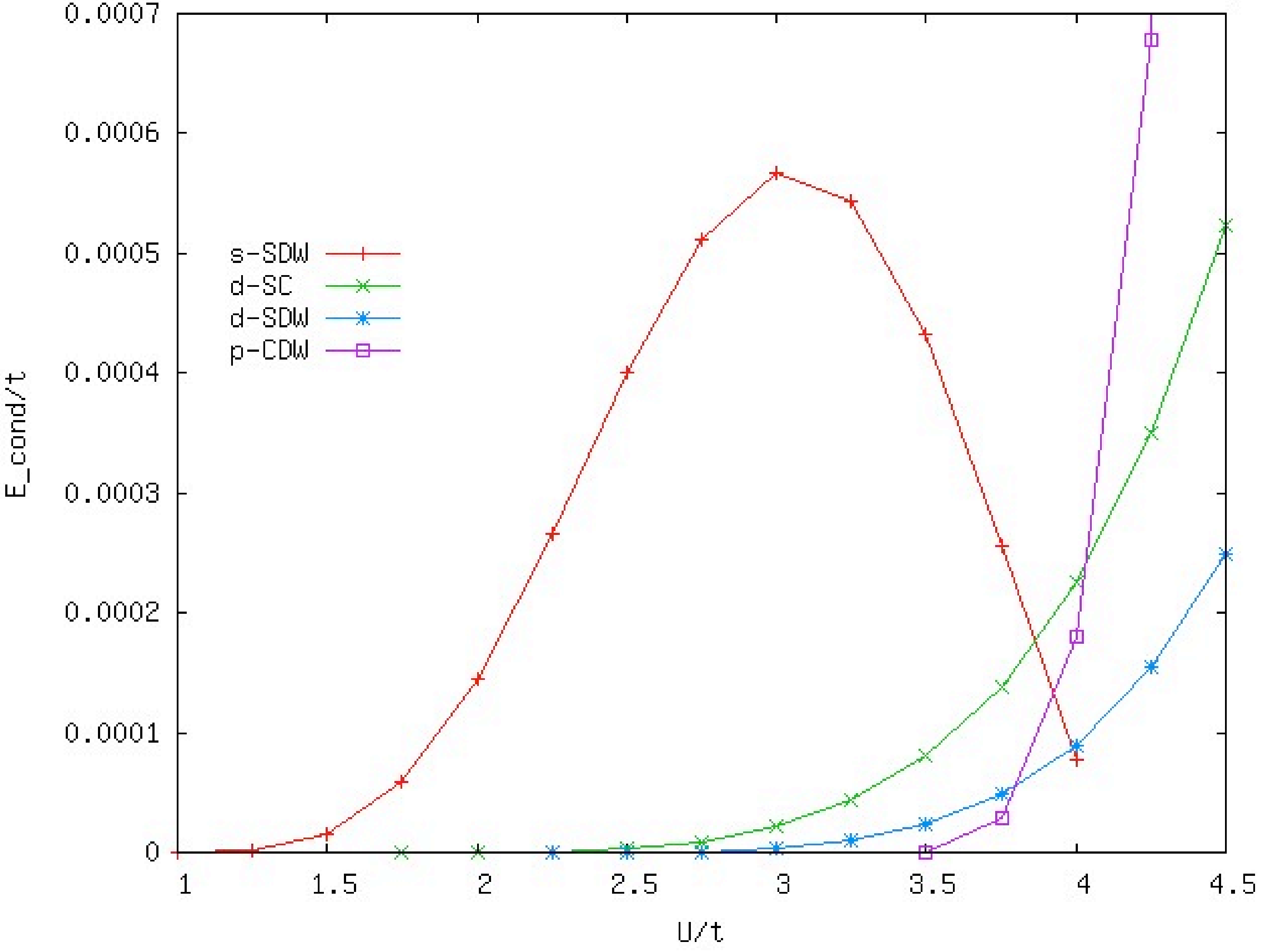
d-SC, d-SDW, d-CDW



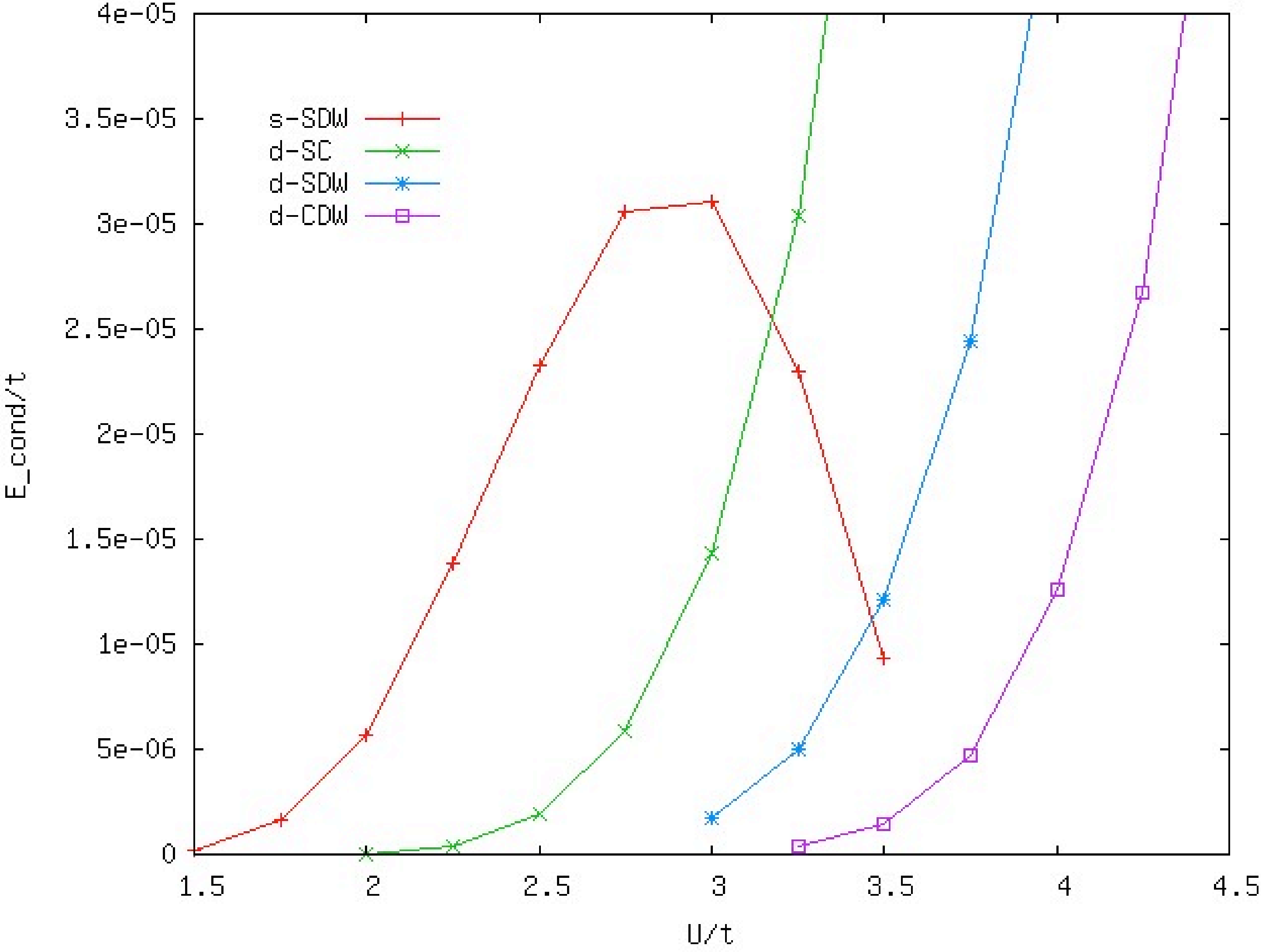
Gap functions for U=3t
t'/t=0, ρ=1, 128x128

Degenerate states
(Hankevych, Wegner)

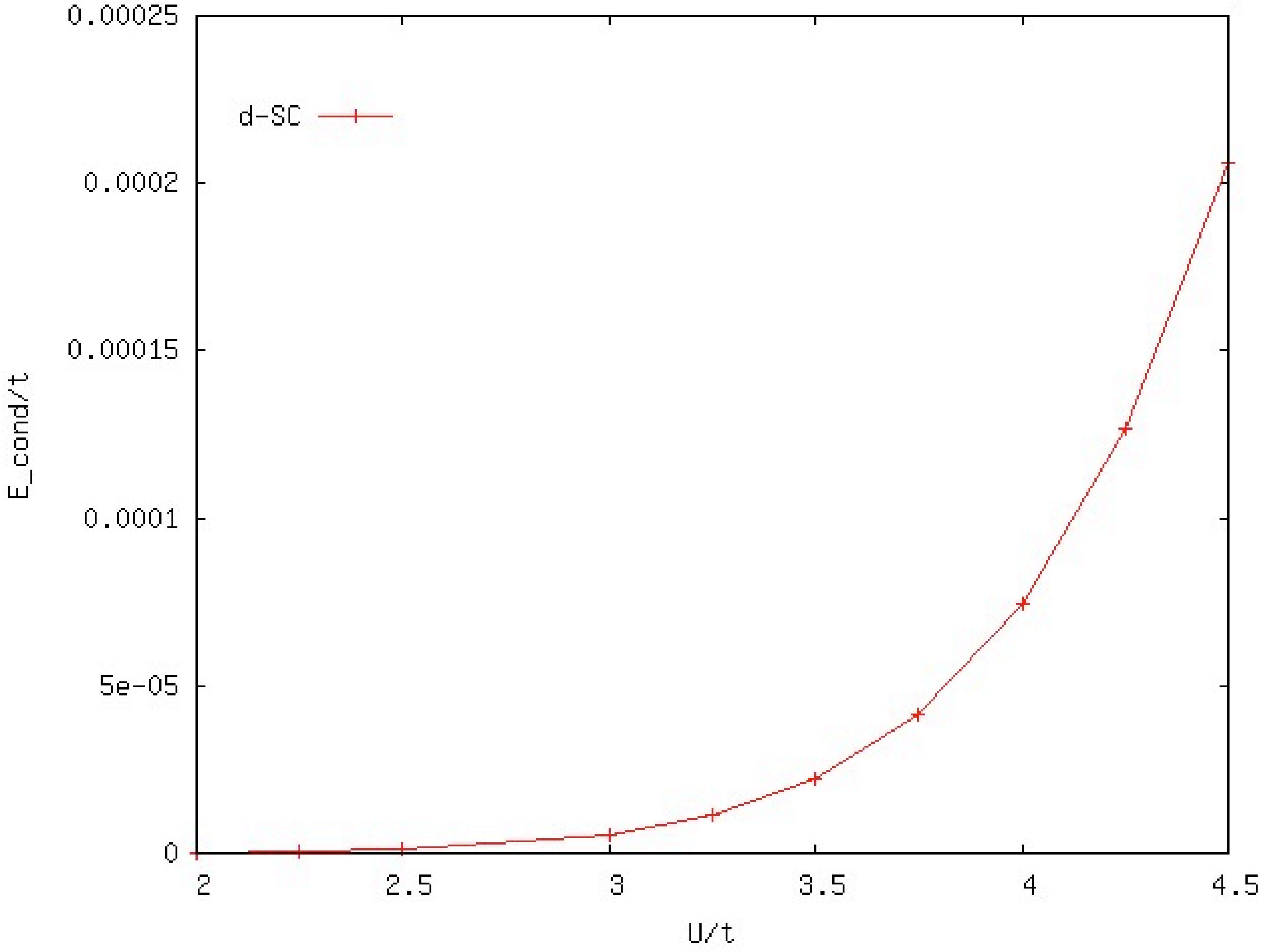
t’/t=0.05, Van Hove density, 128x128



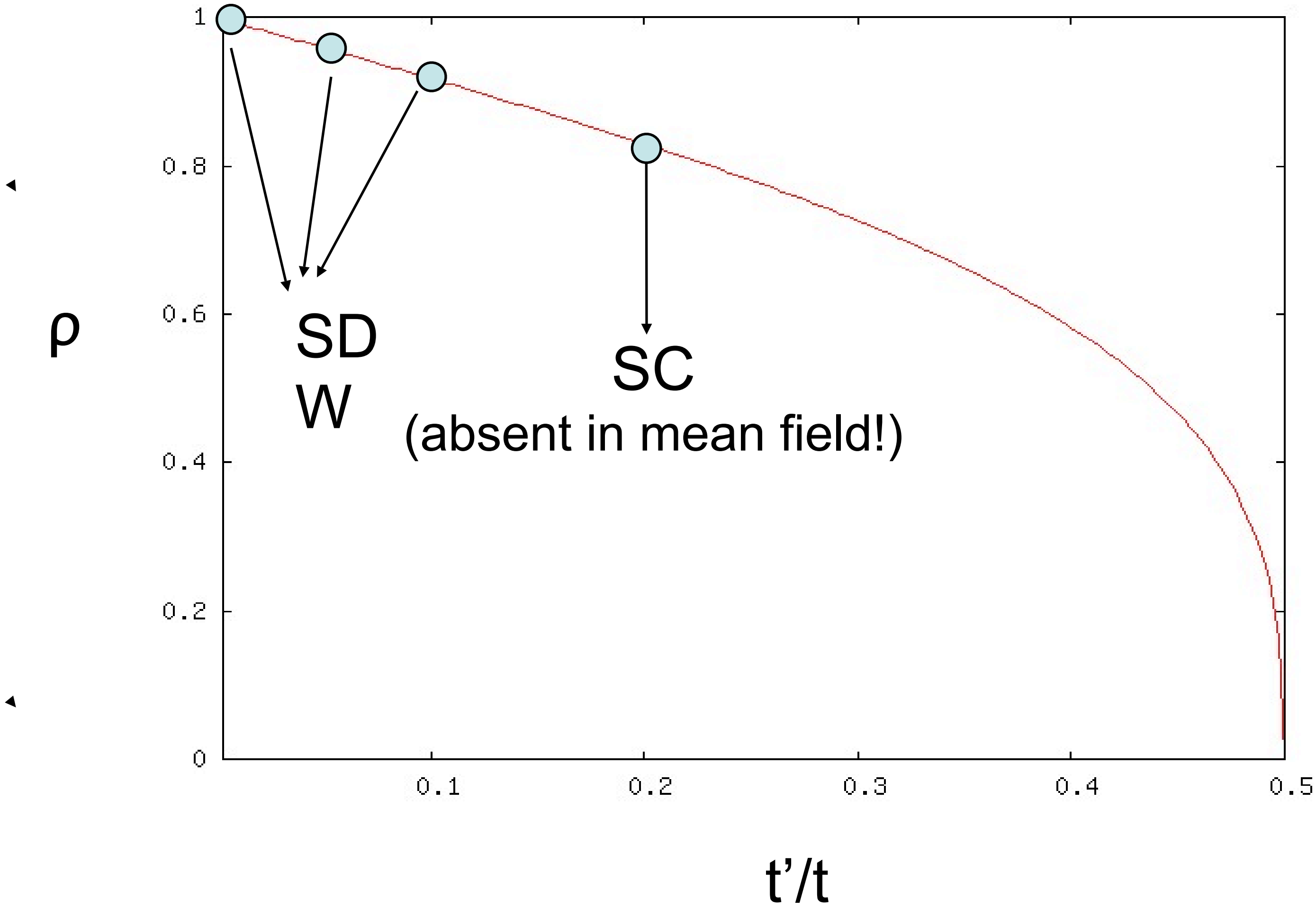
t’/t=0.10, Van Hove density,128x128



t’/t=0.20, Van Hove density, 128x128



Van Hove phase diagram, U=3t



SD
W

SC
(absent in mean field!)

5. Retardation effects

Hubbard-Holstein model

$$
\begin{aligned}
H &= H_{\mathrm{el}} + H_{\mathrm{ph}} + H_1 + H_2 + H_3, \\
H_{\mathrm{el}} &= \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}, \\
H_{\mathrm{ph}} &= \sum_{\mathbf{q}\neq 0} \omega_{\mathbf{q}} a^{\dagger}_{\mathbf{q}} a_{\mathbf{q}}, \\
H_1 &= \frac{U}{L} \sideset{}{'}\sum_{\{123\}} c^{\dagger}_{3\uparrow} c_{1\uparrow} c^{\dagger}_{4\downarrow} c_{2\downarrow} \Delta_{1234}, \\
H_2 &= \frac{U}{L} \sideset{}{'}\sum_{\{123\}} c^{\dagger}_{3\uparrow} c_{1\uparrow} c^{\dagger}_{4\downarrow} c_{2\downarrow} \left(1 - \Delta_{1234}\right), \\
H_3 &= \frac{D}{\sqrt{L}} \sum_{\mathbf{k},\sigma,\mathbf{q}\neq 0} c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k},\sigma} \left(a_{\mathbf{q}} + a^{\dagger}_{-\mathbf{q}}\right),
\end{aligned}
$$

Scattering terms

Eliminate scattering terms: $S = S_e + S_p,$

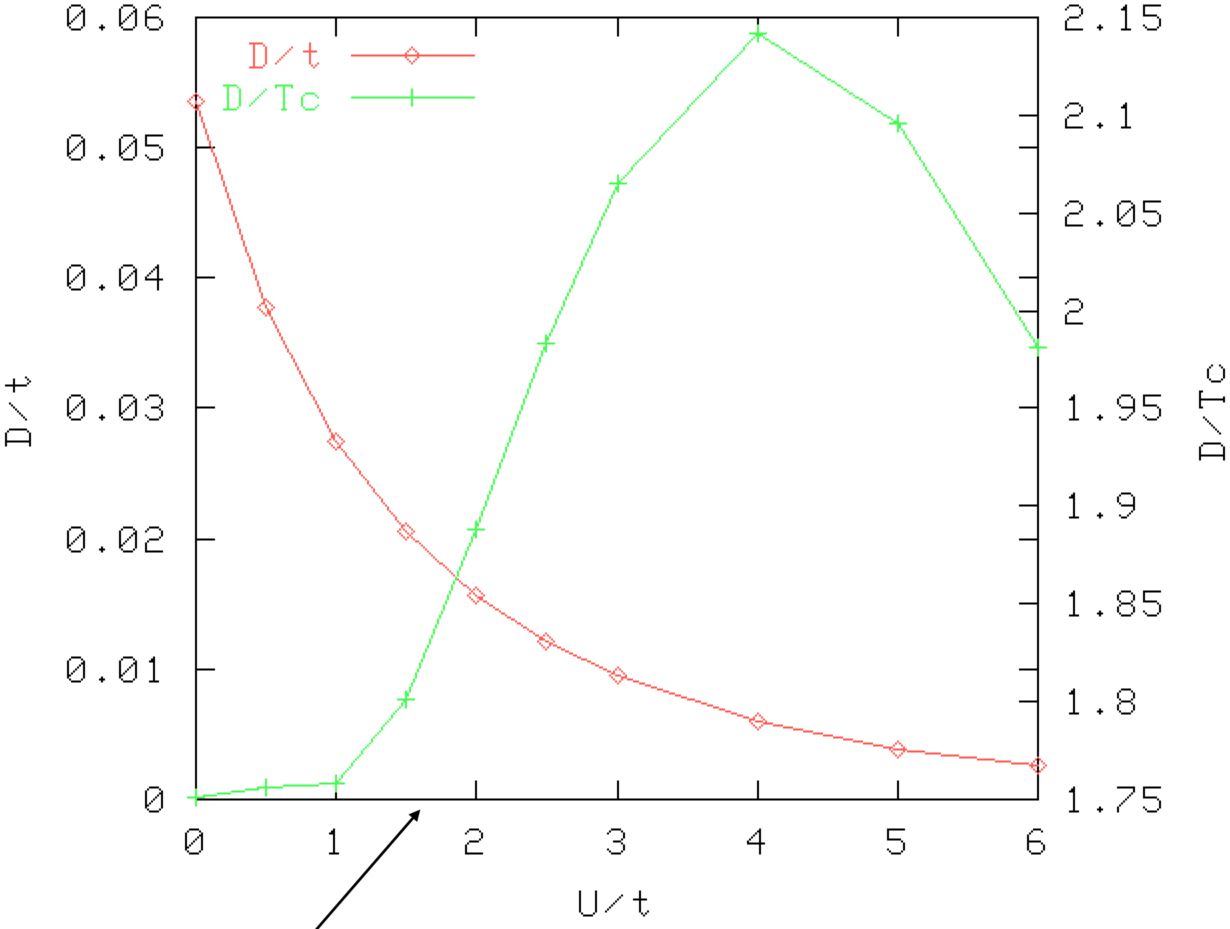
$$S_e = \frac{iU}{L} \sum_{\{123\}}^{\prime} \frac{1 - \Delta_{1234}}{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4} c^\dagger_{3\uparrow} c_{1\uparrow} c^\dagger_{4\downarrow} c_{2\downarrow},$$

$$S_p = \frac{-iD}{\sqrt{L}} \sum_{\mathbf{k},\sigma,\mathbf{q}\neq 0} \left(\frac{c^\dagger_{\mathbf{k+q},\sigma} c_{\mathbf{k},\sigma} a_{\mathbf{q}}}{\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k}} - \omega_{\mathbf{q}}} + \frac{c^\dagger_{\mathbf{k+q},\sigma} c_{\mathbf{k},\sigma} a^\dagger_{-\mathbf{q}}}{\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k}} + \omega_{\mathbf{q}}} \right).$$

Effective interaction in the Cooper channel:

$$V_{\mathbf{kp}} = V^{\mathrm{Hub}}_{\mathbf{kp}} - D^2 \mathrm{Re} \sum_{\sigma=\pm} \frac{\sigma}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}} + \sigma(\omega_{\mathbf{k-p}} + i\Gamma)}$$

D/t=0.4, ω_0/t=0.2, Γ/t=0.02 $\lambda = \frac{2D^2}{\omega_0} N(0) \approx 0.5$

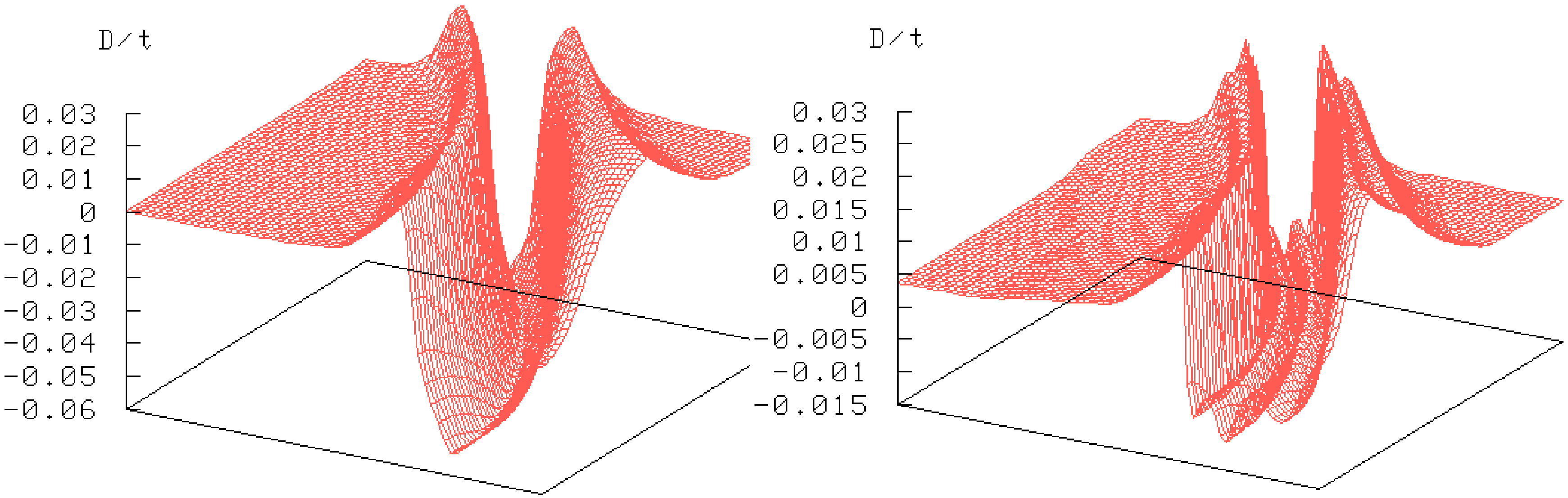


2D^2/ ω_0=1.6t

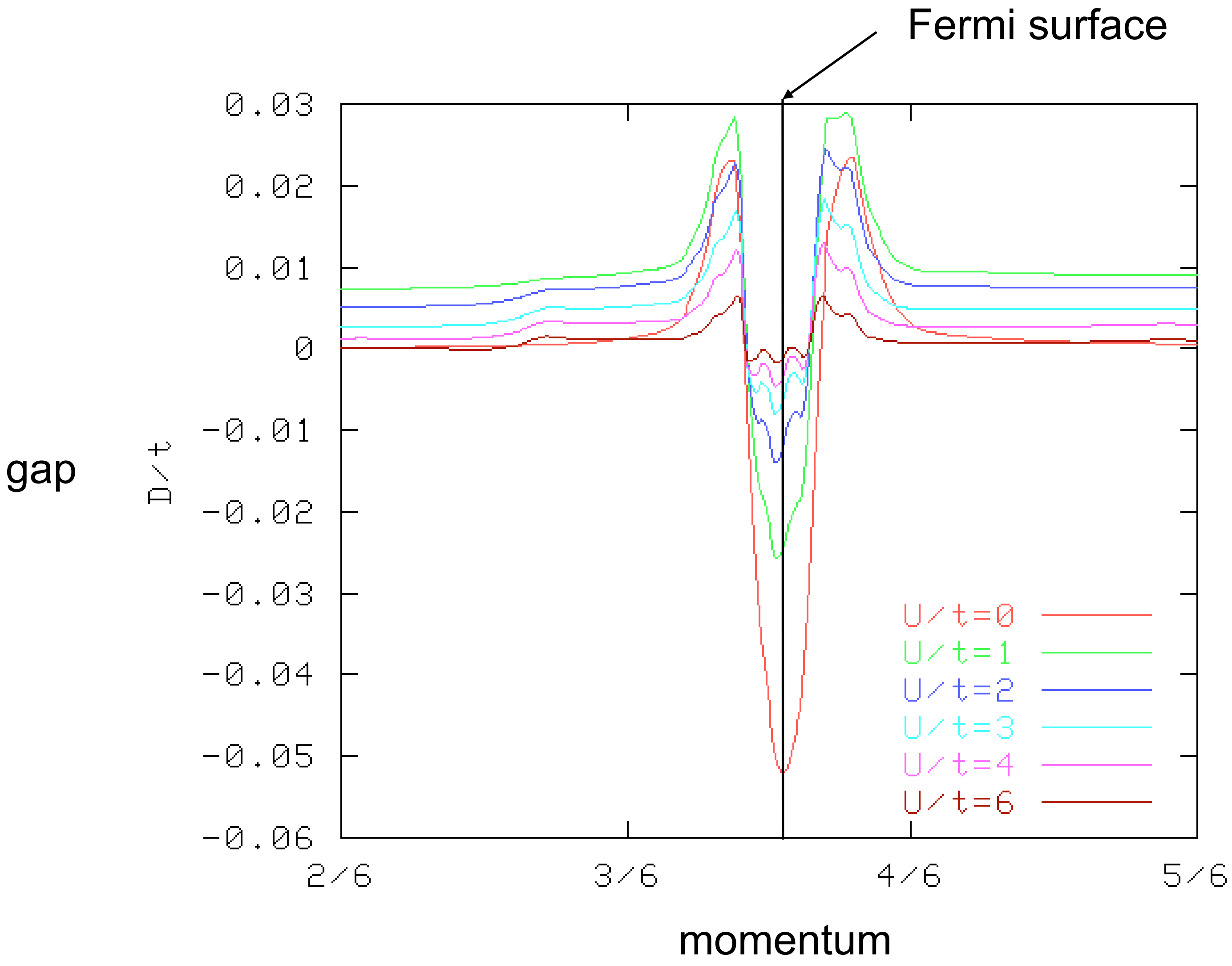
$$\mu^* = \frac{\mu}{1 + \mu \ln\left(\frac{W}{\omega_0}\right)} \rightarrow \frac{1}{\ln\left(\frac{W}{\omega_0}\right)} \approx 0.33$$

Gap function

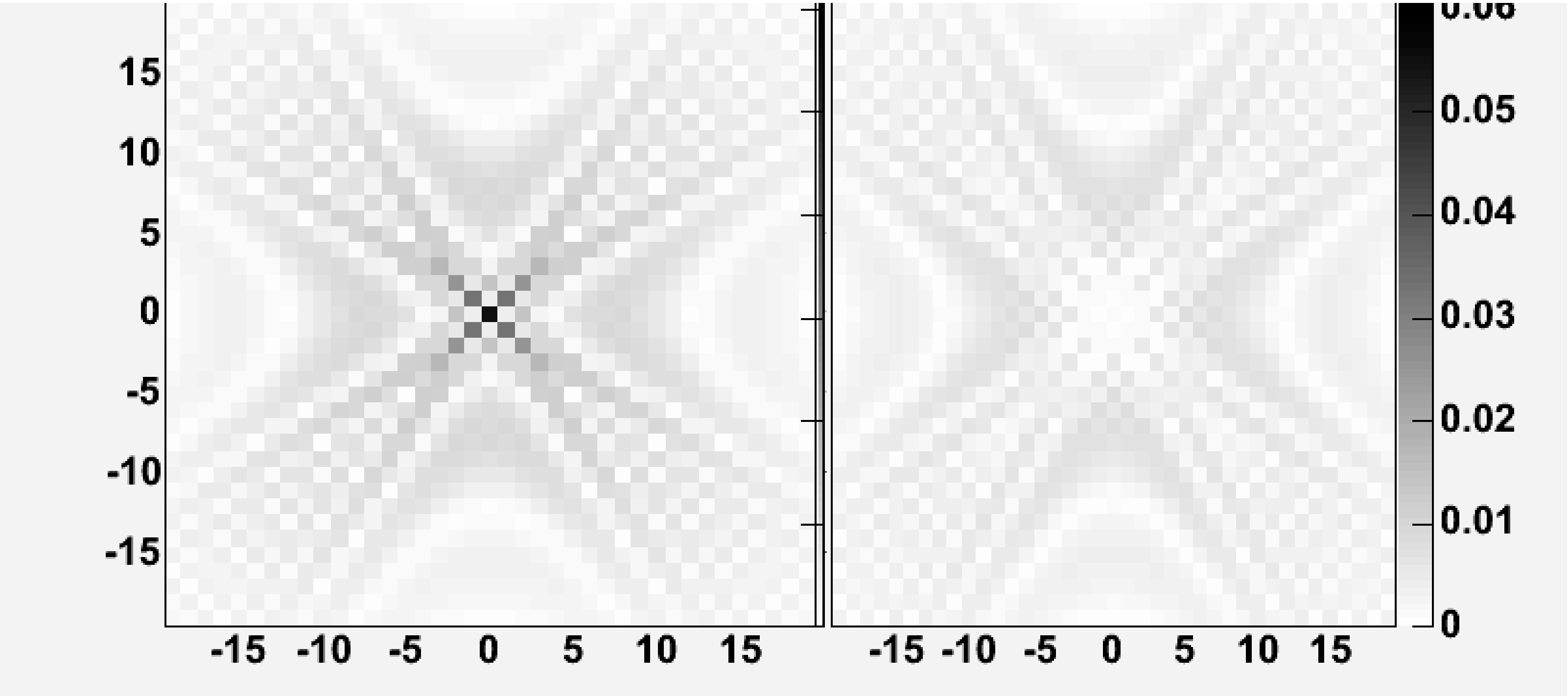
U=0 U=3t



Gap function along (0,0) to (π,π)

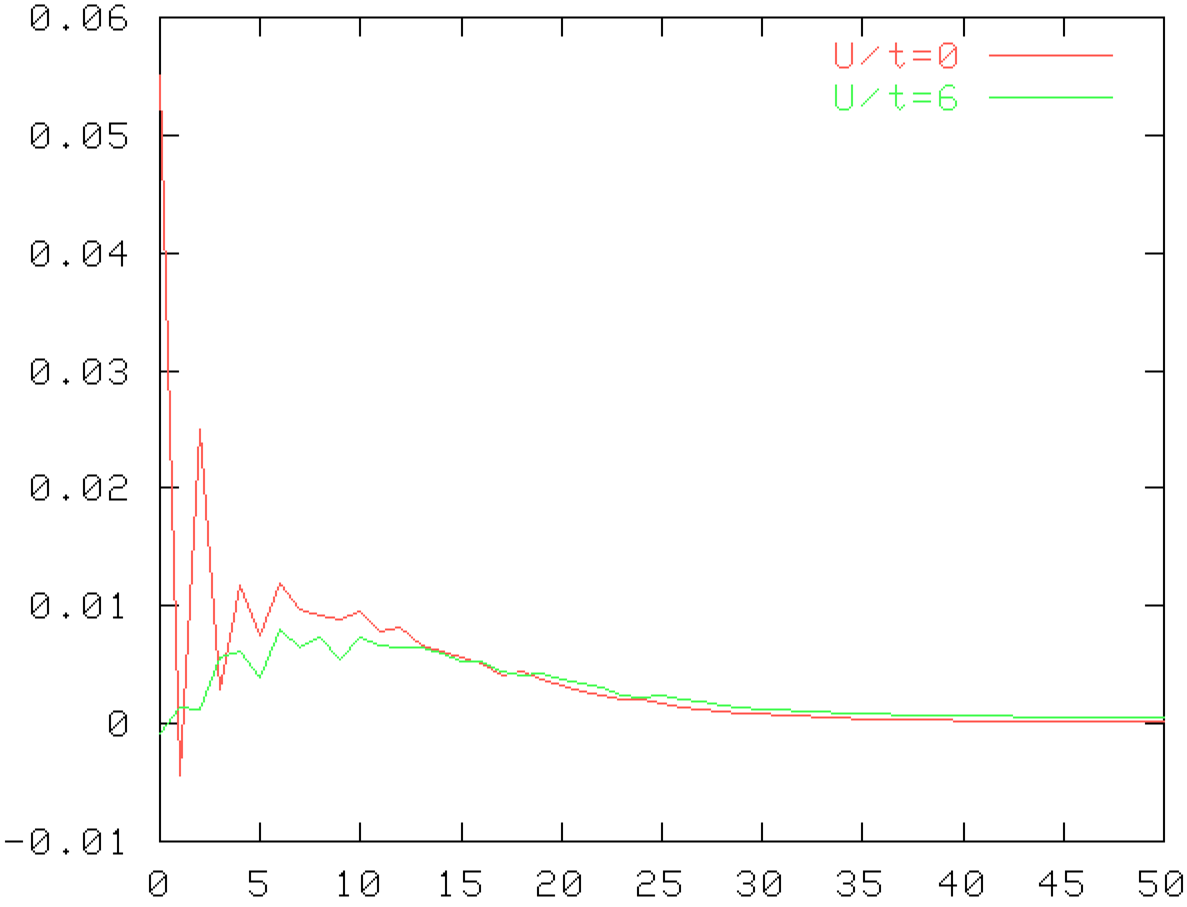


Cooper pair wavefunction



U=0 U=6t

Cooper pair wavefunction



el.-el. distance

Conclusions

- methodology:
- simple 'variational' method allowing comparison of different symmetry breaking patterns on the same footing
- applications:
- fully microscopic model for the T_c enhancement on a bilayer
- t-t' Hubbard model: a possible canonical model for p-wave superconductivity in Sr_2RuO_4
- correlation effects:
- additional structure due to Hubbard U in $\Delta(\omega)$ of the Holstein model
- retardation effects in the d-wave sector: work in progress
- observability of the structure??