Underdoped cuprates phenomenology in the 2D Hubbard model within COM(SCBA)

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CORPES ’07 – April 18, 2007

Outline

1. Composite Operator Method (COM)
   - Philosophy of COM
   - Dyson equation in COM
   - Ingredients of COM

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2. Hubbard Model
   - 2-pole approximation
   - Spin and charge
   - SCBA approximation
3. Cuprates
   - Experiments
   - COM results

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where the composite operators

$$\xi_{\sigma} = \left(1 - c_{\bar{\sigma}}^{\dagger} c_{\bar{\sigma}} \right) c_{\sigma} \qquad \text{and} \qquad \eta_{\sigma} = c_{\bar{\sigma}}^{\dagger} c_{\bar{\sigma}} c_{\sigma}$$

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are eigenoperators of the Hamiltonian

$$\mathrm{i} \frac{\partial}{\partial t} \xi_{\sigma} = [\xi_{\sigma}, H] = -\mu \xi_{\sigma}$$

$$\mathrm{i} \frac{\partial}{\partial t} \eta_{\sigma} = [\eta_{\sigma}, H] = -(\mu - U) \eta_{\sigma}$$

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satisfy non-canonical anti-commutation relations

$\{\xi_\sigma, \xi_{\sigma'}\} = \{\eta_\sigma, \eta_{\sigma'}\} = \{\xi_\sigma^\dagger, \eta_{\sigma'}\} = 0$	$\{\xi_\sigma, \eta_{\sigma'}\} = \delta_{\sigma\bar\sigma'} c_\sigma c_{\bar\sigma}$
$\{\xi_\sigma^\dagger, \xi_{\sigma'}\} = \delta_{\sigma\sigma'}(1 - c_{\bar\sigma}^\dagger c_{\bar\sigma}) + \delta_{\sigma\bar\sigma'} c_\sigma^\dagger c_{\bar\sigma}$	$\{\xi_\sigma^\dagger \xi_\sigma, \xi_{\sigma'}\} = -\delta_{\sigma\sigma'} \xi_\sigma$
$\{\eta_\sigma^\dagger, \eta_{\sigma'}\} = \delta_{\sigma\sigma'} c_{\bar\sigma}^\dagger c_{\bar\sigma} - \delta_{\sigma\bar\sigma'} c_\sigma^\dagger c_{\bar\sigma}$	$\{\eta_\sigma^\dagger \eta_\sigma, \eta_{\sigma'}\} = -\eta_{\sigma'}$
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are the new elementary excitations

c	$\Longrightarrow$	ξ, η
$\downarrow$		$\downarrow$
no more observables!!!		new elementary excitations!!!

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Mancini & Avella; Adv. Phys. **53**, 537 (2004)

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2. $\Delta = \langle \xi^\alpha \xi^\dagger \rangle - \langle \eta^\alpha \eta^\dagger \rangle$

The constraints

1. $n = \langle c^\dagger c \rangle$
2. $\Delta = 0$ Hubbard I

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2. $\Delta = \langle \xi^\alpha \xi^\dagger \rangle - \langle \eta^\alpha \eta^\dagger \rangle$
3. $p = \frac{1}{4}\left(\langle n^\alpha n \rangle + \langle \mathbf{s}^\alpha \mathbf{s} \rangle\right) - \langle \lambda^\alpha \lambda^\dagger \rangle$

The constraints

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2. $\Delta = \langle \xi^\alpha \xi^\dagger \rangle - \langle \eta^\alpha \eta^\dagger \rangle$
3. $p = \frac{1}{4} n^2$ Hubbard I

where $\lambda = c_\uparrow(i) c_\downarrow(i)$

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3. $p \Leftarrow$ 1-loop Roth

where $\lambda = c_\uparrow(i) c_\downarrow(i)$

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4. Summary

The basis: $\psi_\mu = \begin{pmatrix} n_\mu \\ \rho_\mu \end{pmatrix}$ where $n_\mu = (n, \mathbf{s})$ and $-t\rho_\mu = \mathrm{i}\frac{\partial}{\partial t} n_\mu$

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1. $\left\langle \psi^{\alpha_{1,\sqrt{2},2,\sqrt{5},2\sqrt{2}}} \psi^\dagger \right\rangle$

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2. $\left\langle n_\mu n_\mu \right\rangle = n + 2(2\delta_{\mu 0} - 1)D$

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Avella et al.; Phys. Rev. B **67**, 115123 (2003)

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$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF | F^\dagger B^\dagger \rangle\rangle_{\mathrm{irr}} \approx \langle\langle B | B^\dagger \rangle\rangle \langle\langle F | F^\dagger \rangle\rangle$$

The SCBA approximation:

$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF|F^\dagger B^\dagger\rangle\rangle_{\mathrm{irr}} \approx \langle\langle B|B^\dagger\rangle\rangle\langle\langle F|F^\dagger\rangle\rangle$$

The *bosons*: $B = n, \mathbf{s}, \lambda$

The SCBA approximation:

$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF | F^\dagger B^\dagger \rangle\rangle_{\mathrm{irr}} \approxeq \langle\langle B | B^\dagger \rangle\rangle \langle\langle F | F^\dagger \rangle\rangle$$

The *bosons*: $B \approxeq n, \mathbf{s}$

The SCBA approximation:

$\delta J = BF \Rightarrow \Sigma = \langle\langle BF|F^\dagger B^\dagger\rangle\rangle_{\mathrm{irr}} \approx \langle\langle B|B^\dagger\rangle\rangle \langle\langle F|F^\dagger\rangle\rangle$

The *bosons*: $B \approx n, \mathbf{s}$ The *fermions*: $F = \xi, \eta$

The SCBA approximation:

$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF|F^\dagger B^\dagger\rangle\rangle_{\mathrm{irr}} \approx \langle\langle B|B^\dagger\rangle\rangle\langle\langle F|F^\dagger\rangle\rangle$$

The *bosons*: $B \approx n, \mathbf{s}$ The *fermions*: $F = \xi, \eta$

Self-consistency Cycle

$G_0[\mu_0, \Delta_0, p_0]$

The SCBA approximation:

$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF | F^\dagger B^\dagger \rangle\rangle_{\mathrm{irr}} \approx \langle\langle B | B^\dagger \rangle\rangle \langle\langle F | F^\dagger \rangle\rangle$$

The *bosons*: $B \approx n, \mathbf{s}$ The *fermions*: $F = \xi, \eta$

Self-consistency Cycle

$G_0[\mu_0, \Delta_0, p_0]$

↓

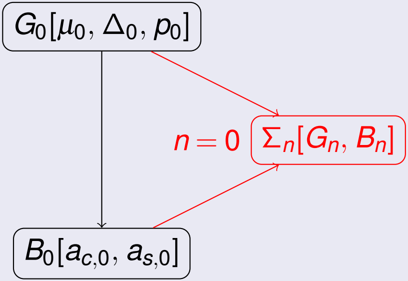
$B_0[a_{c,0}, a_{s,0}]$

The SCBA approximation:

$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF | F^\dagger B^\dagger \rangle\rangle_{\rm irr} \approxeq \langle\langle B | B^\dagger \rangle\rangle \langle\langle F | F^\dagger \rangle\rangle$$

The *bosons*: $B \approxeq n, \mathbf{s}$ The *fermions*: $F = \xi, \eta$

Self-consistency Cycle

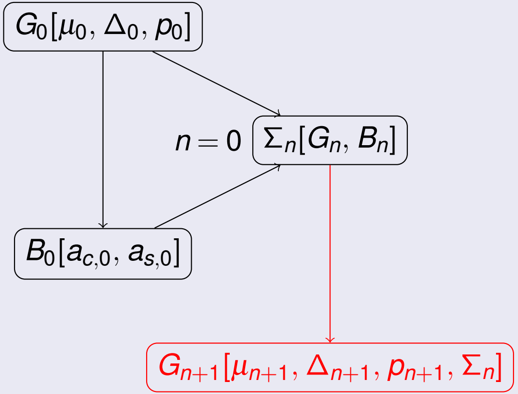


The SCBA approximation:

$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF | F^\dagger B^\dagger \rangle\rangle_{\mathrm{irr}} \approx \langle\langle B | B^\dagger \rangle\rangle \langle\langle F | F^\dagger \rangle\rangle$$

The *bosons*: $B \approx n, \mathbf{s}$ The *fermions*: $F = \xi, \eta$

Self-consistency Cycle

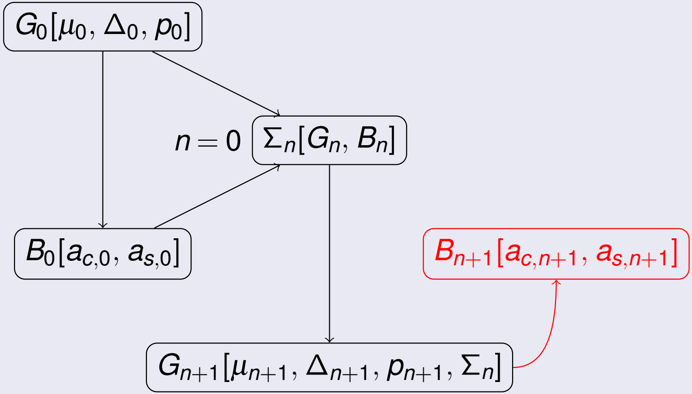


The SCBA approximation:

$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF | F^\dagger B^\dagger \rangle\rangle_{\text{irr}} \approx \langle\langle B | B^\dagger \rangle\rangle \langle\langle F | F^\dagger \rangle\rangle$$

The *bosons*: $B \approx n, \mathbf{s}$ The *fermions*: $F = \xi, \eta$

Self-consistency Cycle

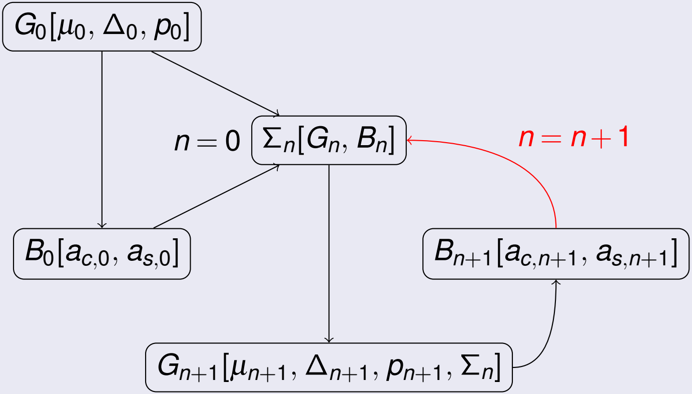


The SCBA approximation:

$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF|F^\dagger B^\dagger\rangle\rangle_{\text{irr}} \approx \langle\langle B|B^\dagger\rangle\rangle \langle\langle F|F^\dagger\rangle\rangle$$

The *bosons*: $B \approx n, \mathbf{s}$ The *fermions*: $F = \xi, \eta$

Self-consistency Cycle

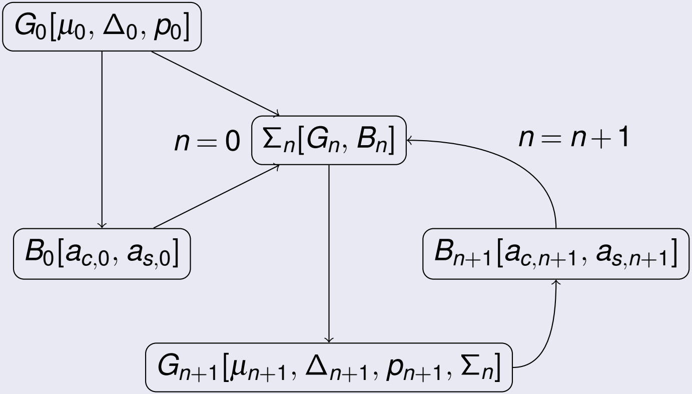


The SCBA approximation:

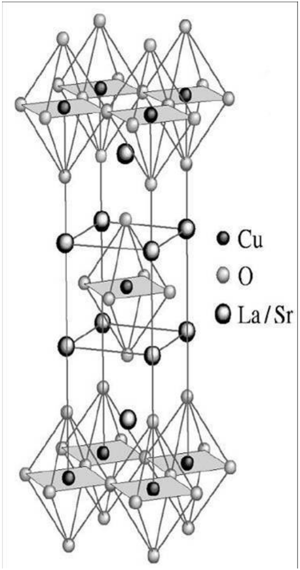
$$\delta J = BF \Rightarrow \Sigma = \langle\langle BF | F^\dagger B^\dagger \rangle\rangle_{\mathrm{irr}} \approx \langle\langle B | B^\dagger \rangle\rangle \langle\langle F | F^\dagger \rangle\rangle$$

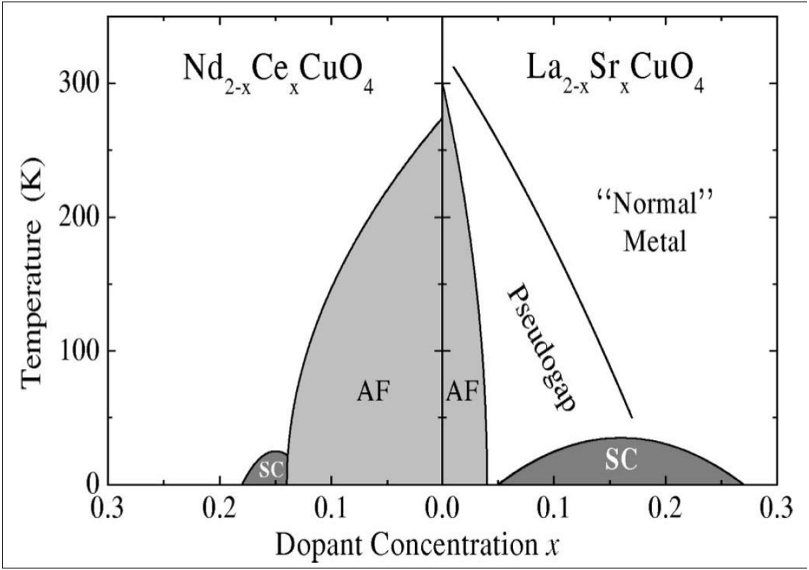
The *bosons*: $B \approxeq n, \mathbf{s}$ The *fermions*: $F = \xi, \eta$

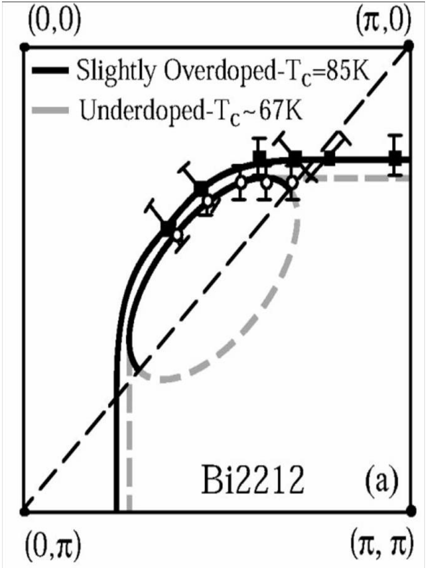
Self-consistency Cycle (Avella & Mancini; Phys. Rev. B **75**, ??? (2007))

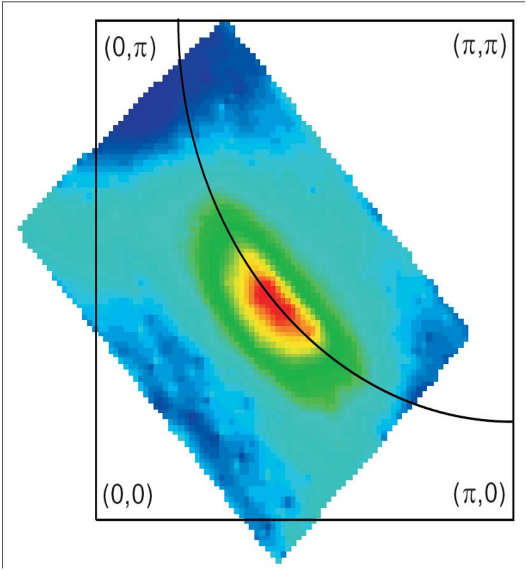


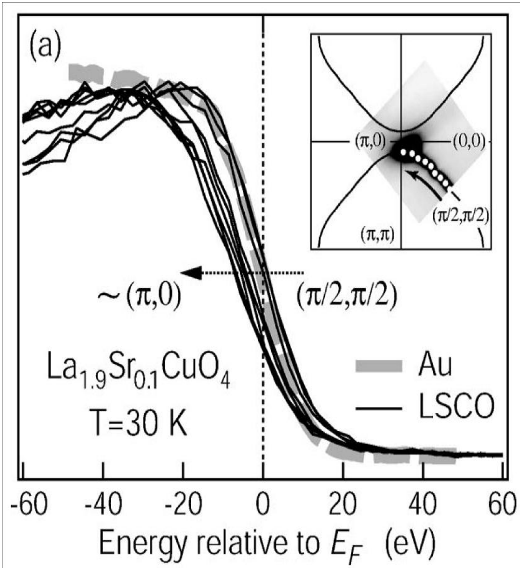
Outline

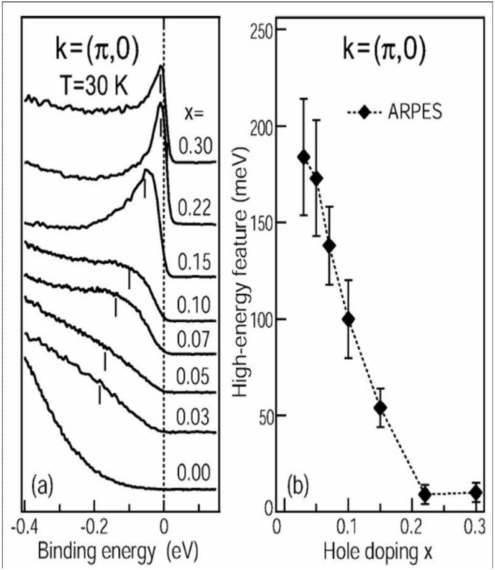

Cu
O
La / Sr

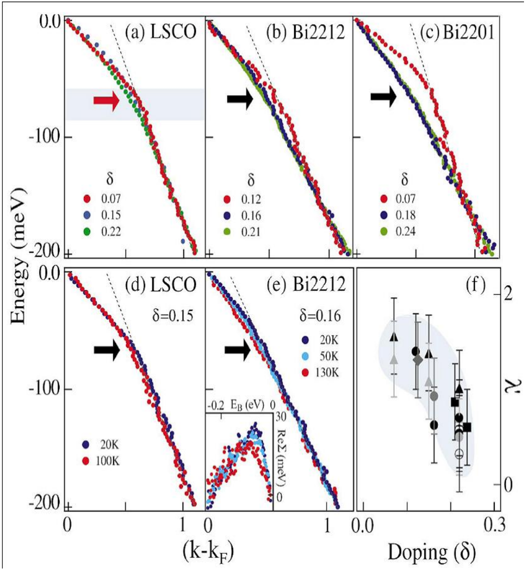

$Nd_{2-x}Ce_xCuO_4$
$La_{2-x}Sr_xCuO_4$
300
200
100
0
Temperature (K)
"Normal"
Metal
Pseudogap
AF
AF
SC
SC
0.3
0.2
0.1
0.0
0.1
0.2
0.3
Dopant Concentration x

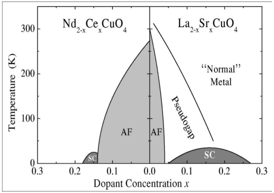

(0,0)
(π,0)
Slightly Overdoped-Tc=85K
Underdoped-Tc~67K
Bi2212
(a)
(0,π)
(π, π)

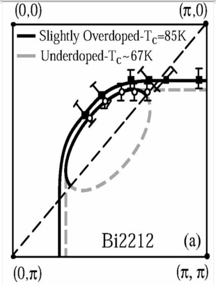

$(0,\pi)$
(π,π)
$(0,0)$
$(\pi,0)$

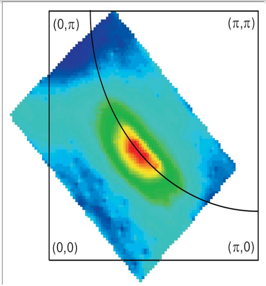

(a)
(π,0)
(0,0)
(π/2,π/2)
(π,π)
~ (π,0)
(π/2,π/2)
$La_{1.9}Sr_{0.1}CuO_4$
T=30 K
Au
LSCO
-60
-40
-20
0
20
40
60
Energy relative to E_F (eV)

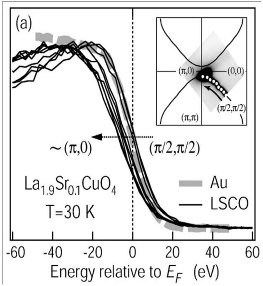

k=(π,0)
T=30 K
x=
0.30
0.22
0.15
0.10
0.07
0.05
0.03
0.00
(a)
-0.4
-0.2
0
Binding energy (eV)
k=(π,0)
ARPES
High-energy feature (meV)
250
200
150
100
50
0
(b)
0
0.1
0.2
0.3
Hole doping x

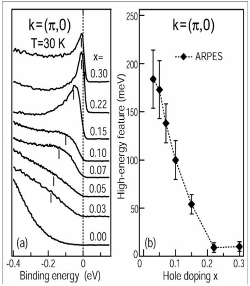

(a) LSCO
(b) Bi2212
(c) Bi2201
(d) LSCO
(e) Bi2212
(f)
δ
0.07
0.15
0.22
0.12
0.16
0.21
0.07
0.18
0.24
δ=0.15
δ=0.16
20K
100K
20K
50K
130K
Energy (meV)
0.0
-100
-200
0
1
(k-k_F)
-0.2 E_B (eV) 0
30
ReΣ (meV)
0.0
0.3
Doping (δ)
2
λ
0

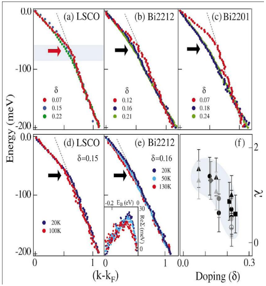

$Nd_{2-x}Ce_xCuO_4$
$La_{2-x}Sr_xCuO_4$
"Normal" Metal
Pseudogap
AF
AF
SC
SC
Temperature (K)
Dopant Concentration x


(0,0)
(π,0)
Slightly Overdoped-T_c=85K
Underdoped-T_c~67K
Bi2212
(a)
(0,π)
(π, π)

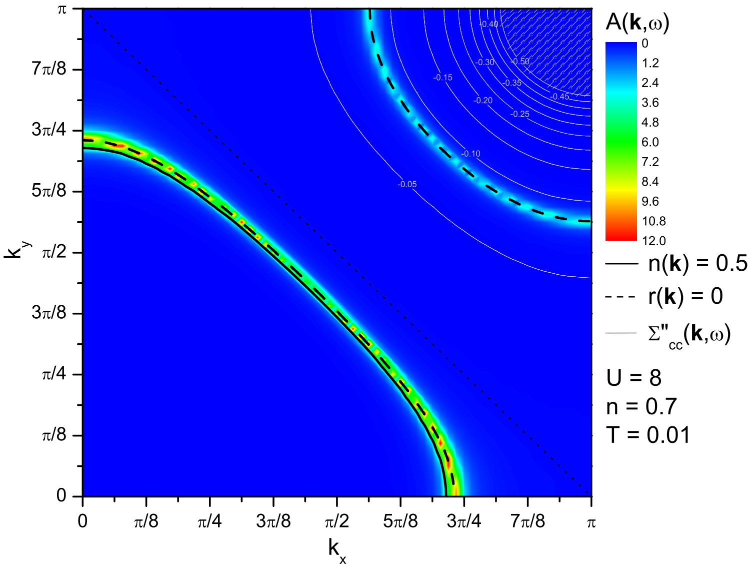

(0,π)
(π,π)
(0,0)
(π,0)

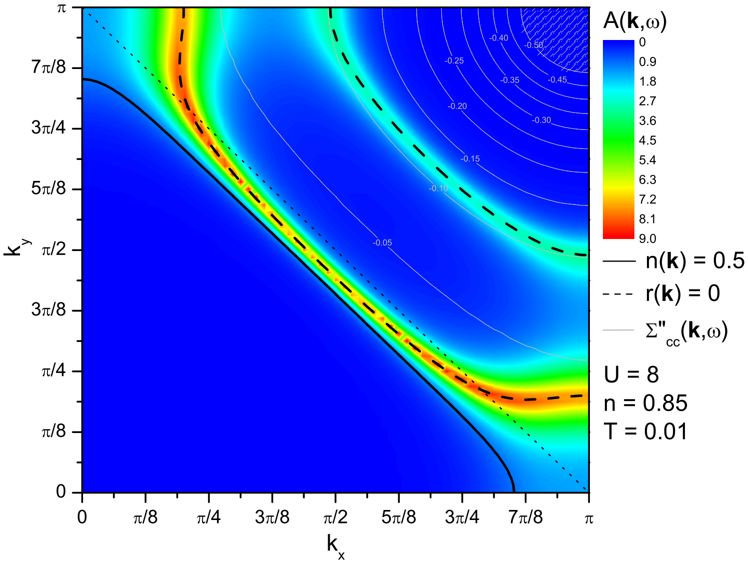

(a)
(π,0)
(0,0)
(π,π)
(π/2,π/2)
~(π,0)
(π/2,π/2)
$La_{1.9}Sr_{0.1}CuO_4$
T=30 K
Au
LSCO
Energy relative to E_F (eV)

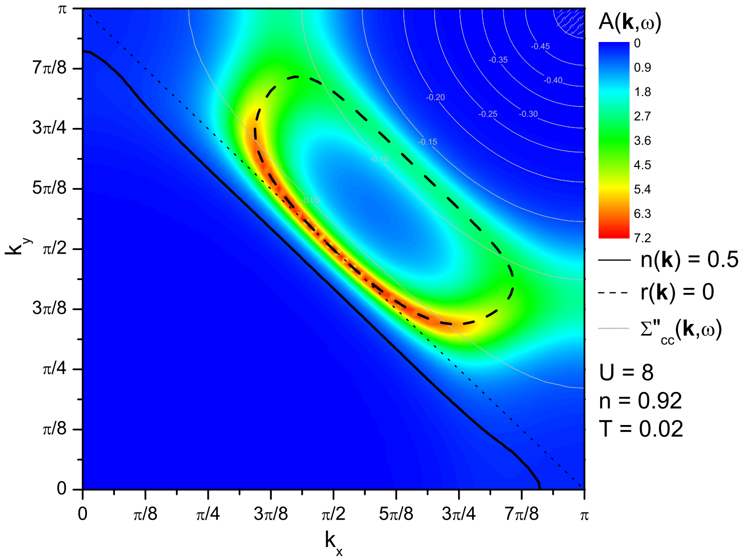

k=(π,0)
T=30 K
x=
0.30
0.22
0.15
0.10
0.07
0.05
0.03
0.00
(a)
Binding energy (eV)
k=(π,0)
ARPES
High-energy feature (meV)
(b)
Hole doping x

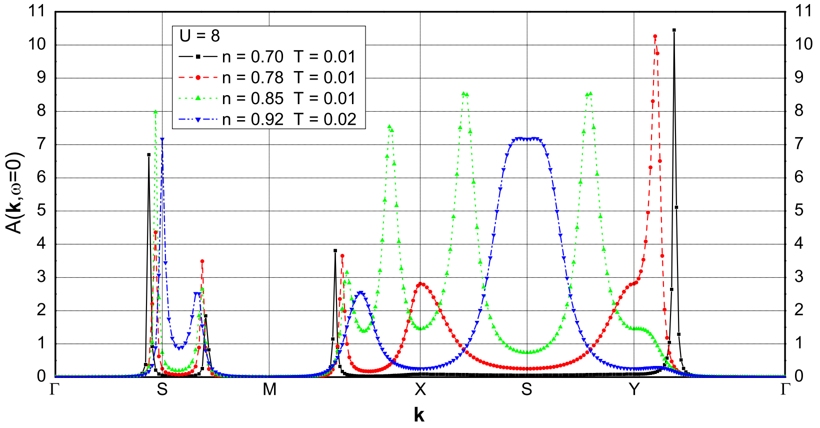

(a) LSCO
(b) Bi2212
(c) Bi2201
(d) LSCO
δ=0.15
(e) Bi2212
δ=0.16
(f)
Energy (meV)
$(k-k_F)$
Doping (δ)

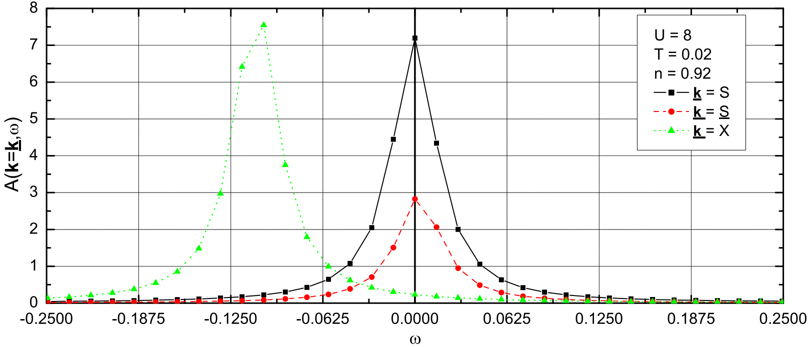
Outline

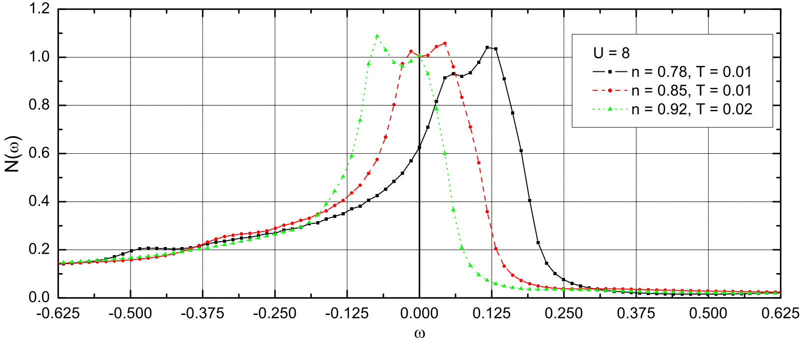

A(k,ω)
0
1.2
2.4
3.6
4.8
6.0
7.2
8.4
9.6
10.8
12.0
n(k) = 0.5
r(k) = 0
Σ"cc(k,ω)
U = 8
n = 0.7
T = 0.01
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
-0.40
-0.45
-0.50
ky
kx
0
π/8
π/4
3π/8
π/2
5π/8
3π/4
7π/8
π


A(k,ω)
0
0.9
1.8
2.7
3.6
4.5
5.4
6.3
7.2
8.1
9.0
n(k) = 0.5
r(k) = 0
Σ"cc(k,ω)
U = 8
n = 0.85
T = 0.01
k_y
k_x
0
π/8
π/4
3π/8
π/2
5π/8
3π/4
7π/8
π
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
-0.40
-0.45
-0.50

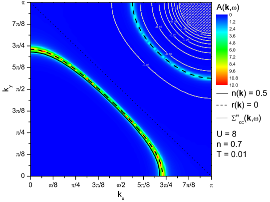

π
7π/8
3π/4
5π/8
π/2
3π/8
π/4
π/8
0
k_y
0 π/8 π/4 3π/8 π/2 5π/8 3π/4 7π/8 π
k_x
-0.45
-0.35
-0.40
-0.20
-0.25
-0.30
-0.15
-0.10
-0.05
A(**k**,ω)
0
0.9
1.8
2.7
3.6
4.5
5.4
6.3
7.2
n(**k**) = 0.5
r(**k**) = 0
Σ"cc(**k**,ω)
U = 8
n = 0.92
T = 0.02

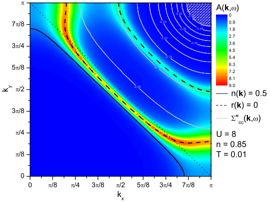

U = 8
n = 0.70 T = 0.01
n = 0.78 T = 0.01
n = 0.85 T = 0.01
n = 0.92 T = 0.02
A(k,ω=0)
k
Γ
S
M
X
S
Y
Γ
0
1
2
3
4
5
6
7
8
9
10
11

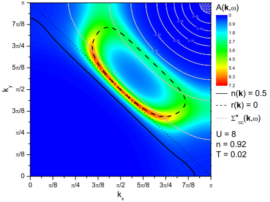

U = 8
T = 0.02
n = 0.92
k = S
k = S
k = X
A(k=k,ω)
ω
0
1
2
3
4
5
6
7
8
-0.2500
-0.1875
-0.1250
-0.0625
0.0000
0.0625
0.1250
0.1875
0.2500

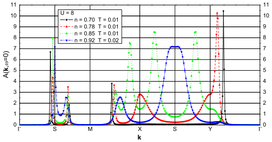

U = 8
n = 0.78, T = 0.01
n = 0.85, T = 0.01
n = 0.92, T = 0.02
N(ω)
ω
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.625
-0.500
-0.375
-0.250
-0.125
0.000
0.125
0.250
0.375
0.500
0.625

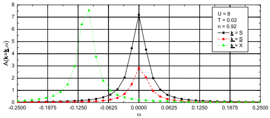
zooms

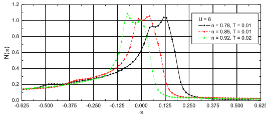

A(k,ω)
n(k) = 0.5
r(k) = 0
Σ''cc(k,ω)
U = 8
n = 0.7
T = 0.01
ky
kx

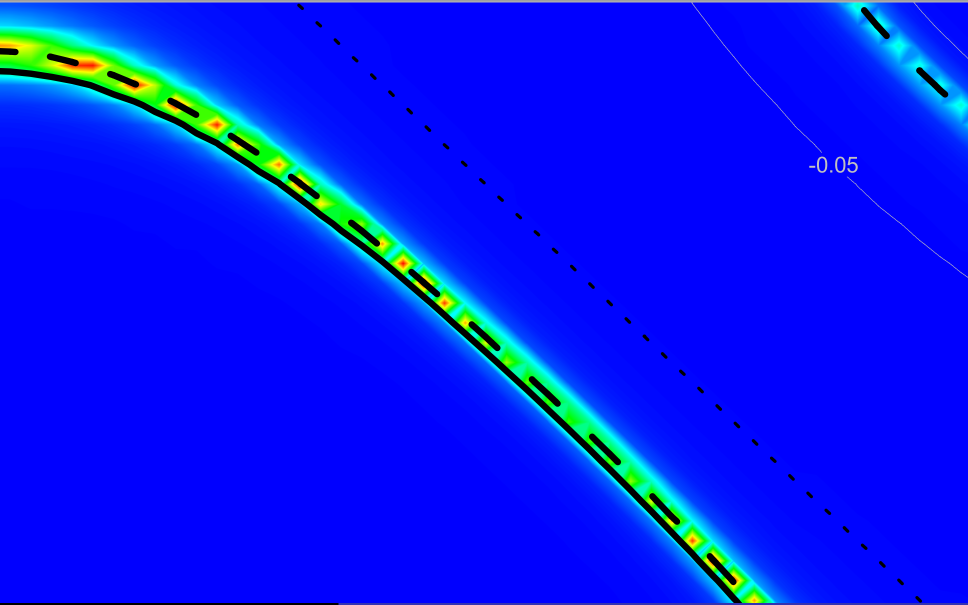

A(k,ω)
n(k) = 0.5
r(k) = 0
Σ''cc(k,ω)
U = 8
n = 0.85
T = 0.01
ky
kx

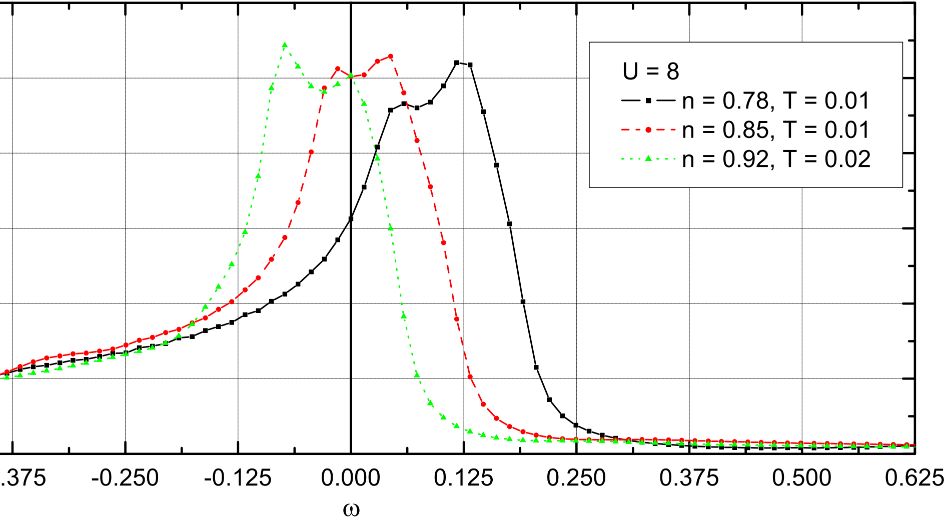

A(k,ω)
n(k) = 0.5
r(k) = 0
Σ''cc(k,ω)
U = 8
n = 0.92
T = 0.02
ky
kx

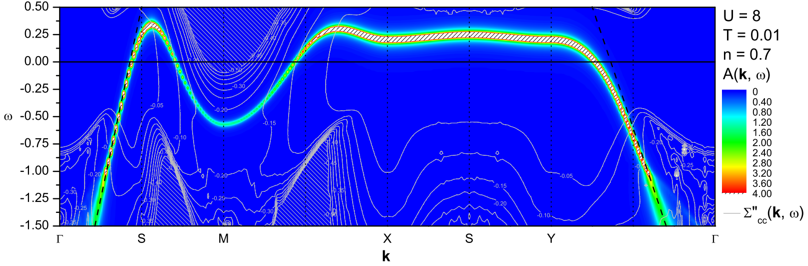

U = 8
n = 0.70 T = 0.01
n = 0.78 T = 0.01
n = 0.85 T = 0.01
n = 0.92 T = 0.02
A(k,ω=0)
k

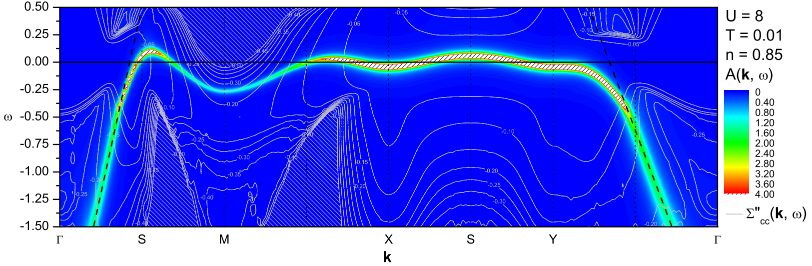

U = 8
T = 0.02
n = 0.92
k = S
k = S
k = X
ω

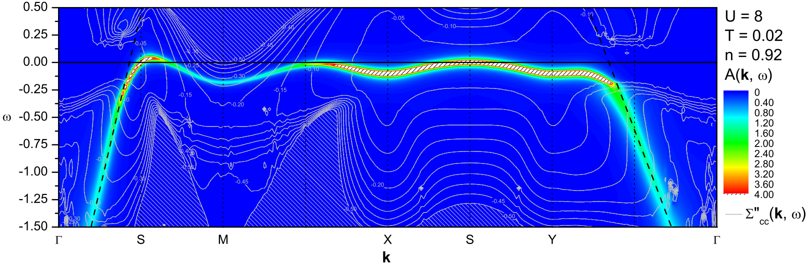

U = 8
n = 0.78, T = 0.01
n = 0.85, T = 0.01
n = 0.92, T = 0.02
N(ω)
ω

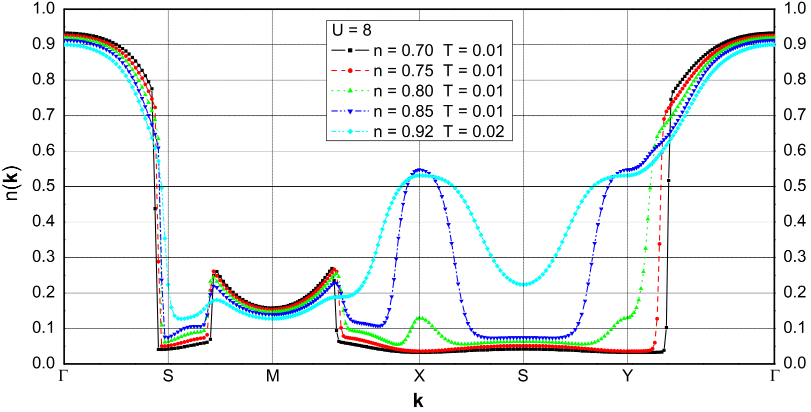

-0.05

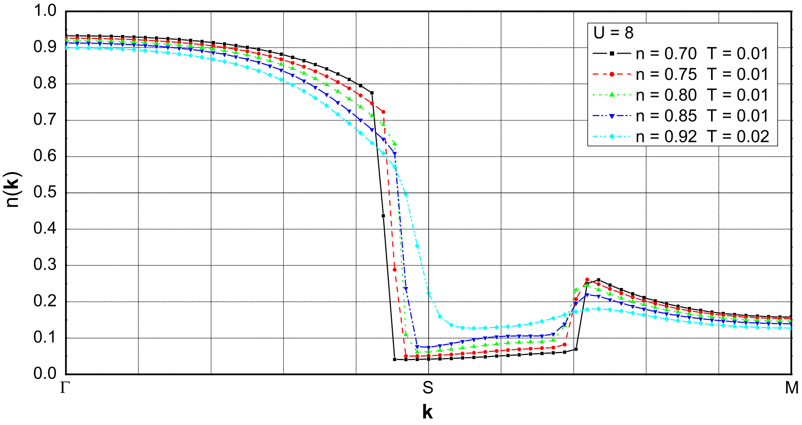

U = 8
n = 0.78, T = 0.01
n = 0.85, T = 0.01
n = 0.92, T = 0.02
.375
-0.250
-0.125
0.000
0.125
0.250
0.375
0.500
0.625
ω

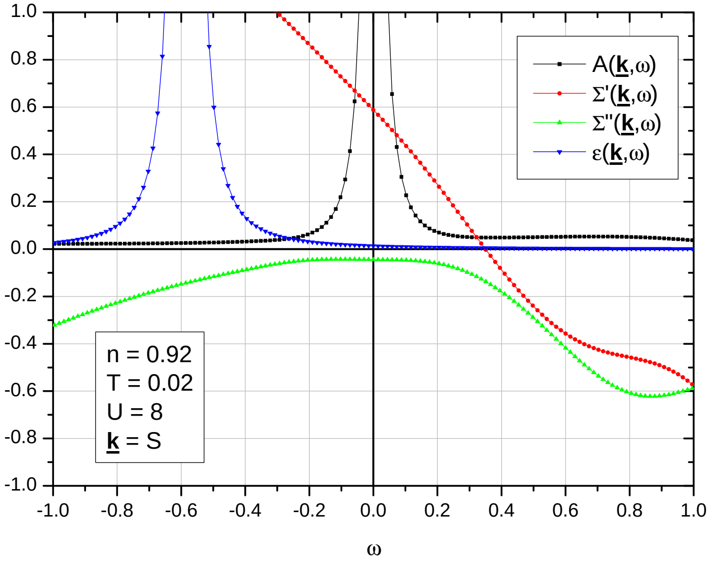

0.50
0.25
0.00
-0.25
-0.50
-0.75
-1.00
-1.25
-1.50
ω
Γ
S
M
X
S
Y
Γ
k
U = 8
T = 0.01
n = 0.7
A(k, ω)
0
0.40
0.80
1.20
1.60
2.00
2.40
2.80
3.20
3.60
4.00
Σ"cc(k, ω)

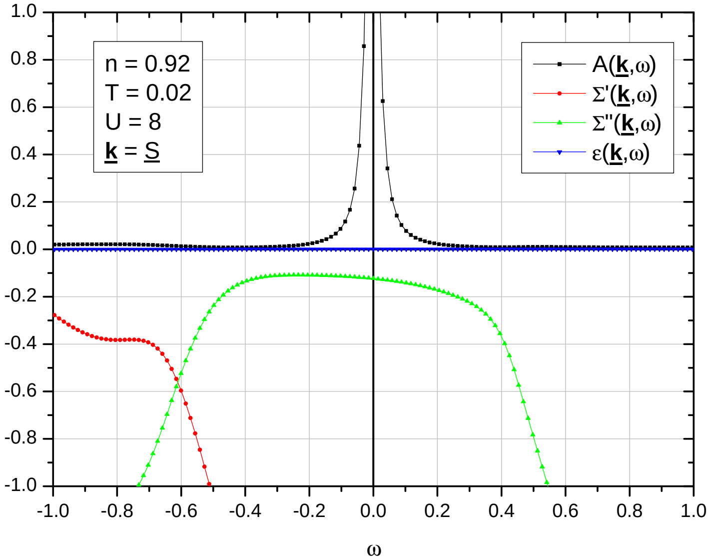

0.50
0.25
0.00
-0.25
ω -0.50
-0.75
-1.00
-1.25
-1.50
Γ
S
M
X
S
Y
Γ
k
U = 8
T = 0.01
n = 0.85
A(k, ω)
0
0.40
0.80
1.20
1.60
2.00
2.40
2.80
3.20
3.60
4.00
Σ"cc(k, ω)

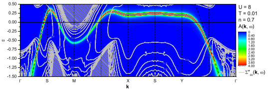

U = 8
T = 0.02
n = 0.92
A(k, ω)
Σ"cc(k, ω)
ω
k
Γ
S
M
X
S
Y
Γ
0.50
0.25
0.00
-0.25
-0.50
-0.75
-1.00
-1.25
-1.50
0
0.40
0.80
1.20
1.60
2.00
2.40
2.80
3.20
3.60
4.00

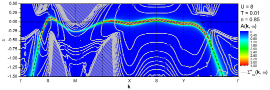

U = 8
n = 0.70 T = 0.01
n = 0.75 T = 0.01
n = 0.80 T = 0.01
n = 0.85 T = 0.01
n = 0.92 T = 0.02
n(k)
k
Γ
S
M
X
S
Y
Γ
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0

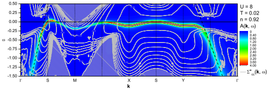

U = 8
n = 0.70 T = 0.01
n = 0.75 T = 0.01
n = 0.80 T = 0.01
n = 0.85 T = 0.01
n = 0.92 T = 0.02
n(k)
k
Γ
S
M
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0

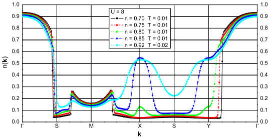

A(k,ω)
Σ'(k,ω)
Σ''(k,ω)
ε(k,ω)
n = 0.92
T = 0.02
U = 8
k = S
ω
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.0 -0.8 -0.6 -0.4 -0.2 0.0 0.2 0.4 0.6 0.8 1.0

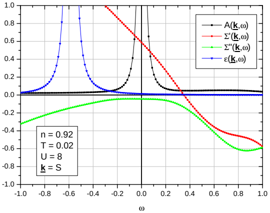

n = 0.92
T = 0.02
U = 8
k = S
A(k,ω)
Σ'(k,ω)
Σ''(k,ω)
ε(k,ω)
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.0 -0.8 -0.6 -0.4 -0.2 0.0 0.2 0.4 0.6 0.8 1.0
ω

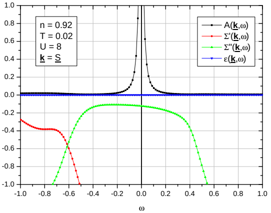

U = 8
T = 0.01
n = 0.7
A(k, ω)
Σ''cc(k, ω)
ω
Γ S M X S Y Γ
k


U = 8
T = 0.01
n = 0.85
A(k, ω)
Σ''cc(k, ω)
ω
Γ S M X S Y Γ
k


U = 8
T = 0.02
n = 0.92
A(k, ω)
Σ''cc(k, ω)
ω
Γ S M X S Y Γ
k


U = 8
n = 0.70 T = 0.01
n = 0.75 T = 0.01
n = 0.80 T = 0.01
n = 0.85 T = 0.01
n = 0.92 T = 0.02
n(k)
Γ S M X S Y Γ
k


A(k,ω)
Σ'(k,ω)
Σ''(k,ω)
ε(k,ω)
n = 0.92
T = 0.02
U = 8
k = S
ω


n = 0.92
T = 0.02
U = 8
k = S
A(k,ω)
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ε(k,ω)
ω

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- Kinks have been found in the dispersion along nodal and anti-nodal directions.
- A properly microscopically derived susceptibility can give results practically identical or, at least, very similar to those attainable by means of phenomenological susceptibilities specially tailored to describe experiments.

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Thank you for your attention!