Variational Cluster Perturbation Theory
and
Superconductivity in the Hubbard Model

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DÉPARTEMENT de PHYSIQUE

d-SC in the Hubbard model ?

- Dynamical cluster approximation (DCA)
  Th. Maier, M. Jarrell, Th. Pruschke, and J. Keller PRL **85**, 1524 (2000)
  Th. Maier et al., cond-mat/0504529

- Exact diagonalizations
  D. Poilblanc and D.J. Scalapino Phys. Rev. **B** 66, 052513 (2002)

- Variational wavefunctions
  A. Paramekanti, Mohit Randeria, and Nandini Trivedi, PRL 87, 217002 (2001)
  S. Sorella et al., PRL **88**, 117002 (2002)

- Variational Cluster Perturbation Theory
  D. Sénéchal, P.-L. Lavertu, M.-A. Marois and A.-M.S. Tremblay, PRL **94**, 156404 (2005)
  M. Aichorn and E. Arrigoni, cond-mat/0502047
  W. Hanke et al., cond-mat/0506364

- Cluster Dynamical Mean Field Theory (CDMFT)
  S. Kancharla et al., (in preparation)

Review : Th. Maier, M. Jarrell, Th. Pruschke, M.H. Hettler, RMP (2005)

Outline

1. Variational Cluster Perturbation Theory

2. Computational details

3. Interplay of Antiferromagnetism and d-wave superconductivity

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Self-energy functional Theory

M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

Dynamic variational principle:

$$\frac{\delta\Omega_t[\Sigma]}{\delta\Sigma} = 0 \quad \Longrightarrow \quad \frac{\partial\Omega_t(h)}{\partial h} = 0$$

$$\Omega_t[\Sigma] = F[\Sigma] - \mathrm{Tr}\ln(G_0^{-1} - \Sigma)$$

Universality of F:

$$\Omega_t[\Sigma] + \mathrm{Tr}\ln(G_0^{-1} - \Sigma) = \Omega_{t'}[\Sigma] + \mathrm{Tr}\ln(G_0'^{-1} - \Sigma)$$

Lattice vs reference Hamiltonian: differ in their 1-body terms

$$H = \sum_{\alpha,\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} \qquad H' : t_{\alpha\beta} \to t'_{\alpha\beta}$$

Restrict Σ to exact self-energy of reference system H'

$$\Omega_t[\Sigma] = \Omega' - \mathrm{Tr}\ln\left[1 + (G_0^{-1} - G_0'^{-1})G'\right]$$

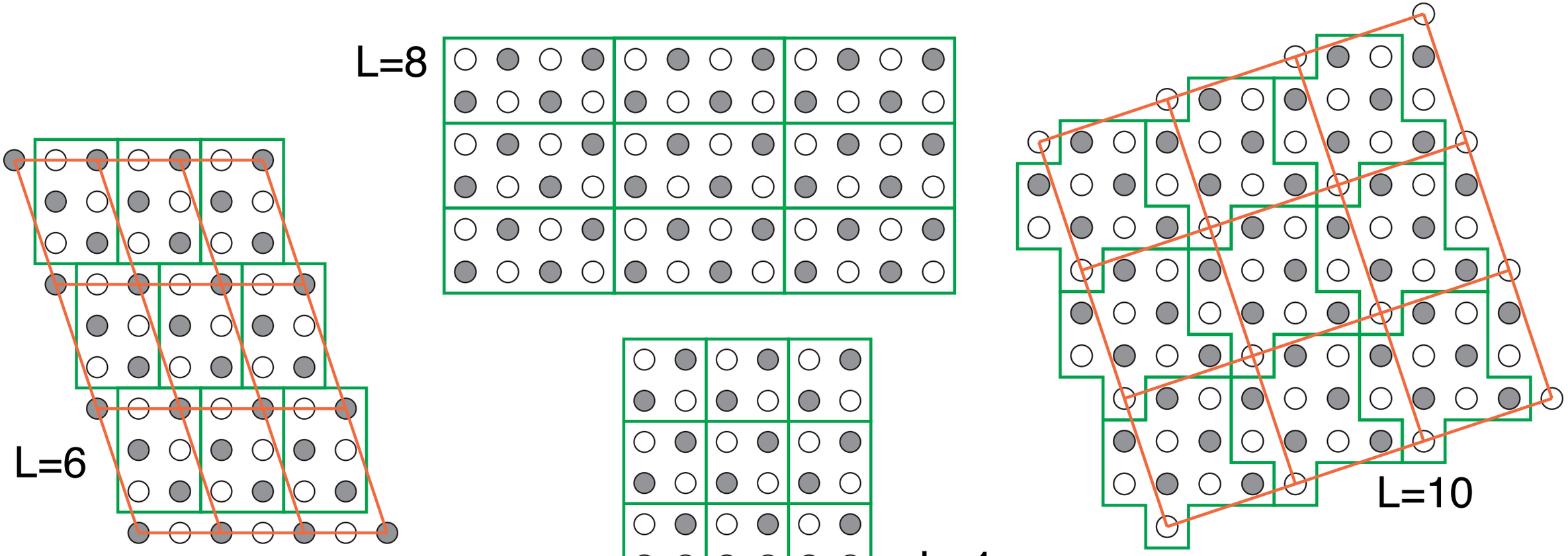
Variational Cluster Approach (VCA, VCPT)

Reference system : isolated cluster

Dahnken et al., Phys. Rev. B 70, 245110 (2004).

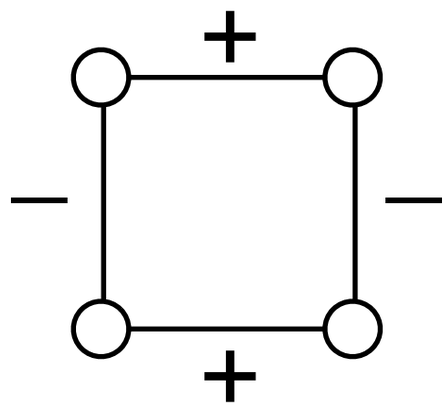
Sénéchal et al., Phys. Rev. Lett. 94, 156404 (2005).

$$
\begin{aligned}
H' \quad = \quad & \sum_{\mathbf{x},\mathbf{x}',\sigma} t_{\mathbf{x}\mathbf{x}'} c^\dagger_{\mathbf{x}\sigma} c_{\mathbf{x}'\sigma} - M \sum_{\mathbf{x},\sigma} \mathrm{e}^{i\mathbf{Q}\cdot\mathbf{x}} (-1)^\sigma n_{\mathbf{x}\sigma} \\
& - \sum_{\mathbf{x},\mathbf{x}'} \left(\Delta_{\mathbf{x}\mathbf{x}'} c_{\mathbf{x}\uparrow} c_{\mathbf{x}'\downarrow} + \mathrm{H.c.} \right) - \mu \sum_{\mathbf{x},\sigma} n_{\mathbf{x}\sigma} + U \sum_{\mathbf{x}} n_{\mathbf{x}\uparrow} n_{\mathbf{x}\downarrow}
\end{aligned}
$$



Nambu formalism

Singlet d-wave Weiss field:



Particle-hole transformation on the down spins:

$$c_{i,1} = c_{i\uparrow} \qquad c_{i,2} = c^{\dagger}_{i\downarrow}$$

Example: hopping matrix of 2-site cluster:

$$\hat{t} = \left(\begin{array}{cc|cc} U-\mu-M & -t & 0 & -\Delta \\ -t & U-\mu+M & -\Delta & 0 \\ \hline 0 & -\Delta & \mu-M & t \\ -\Delta & 0 & t & M \end{array}\right)$$

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Cluster vs lattice Green functions

Zero-temperature cluster Green function:

$$G'_{\alpha\beta}(z) = \langle\Omega|c_\alpha \frac{1}{z - H' + E'_0} c^\dagger_\beta|\Omega\rangle + \langle\Omega|c^\dagger_\beta \frac{1}{z + H' - E'_0} c_\alpha|\Omega\rangle$$

- Computed with the Lanczos method.
- Continued fraction representation stored.
- Easily computed for any complex frequency z

Approximate (periodized) lattice Green function:

$$G(\mathbf{k},\omega) = \frac{1}{L}\sum_{\mathbf{x},\mathbf{x}'} \mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \left(\frac{1}{G_0^{-1}(\mathbf{k},\omega) - \Sigma(\omega)}\right)_{\mathbf{x}\mathbf{x}'}$$

Calculation of the functional

$$\Omega_t[\Sigma] = \Omega' - \mathrm{Tr}\ln\left[1 + (G_0^{-1} - {G'_0}^{-1})G'\right]$$

$$\Omega_t[\Sigma] = \Omega' - \int_{\mathrm{Im}+} \frac{\mathrm{d}\omega}{\pi} \sum_{\mathbf{K}} \ln\det\left[1 + (\hat{t}(\mathbf{K}) - \hat{t}')\hat{G}'(\omega)\right]$$

Integral along positive imaginary axis (convergent)

Cluster Green function

Cluster ground state energy

Summation over reduced Brillouin zone

Lattice model hopping matrix

cluster hopping matrix

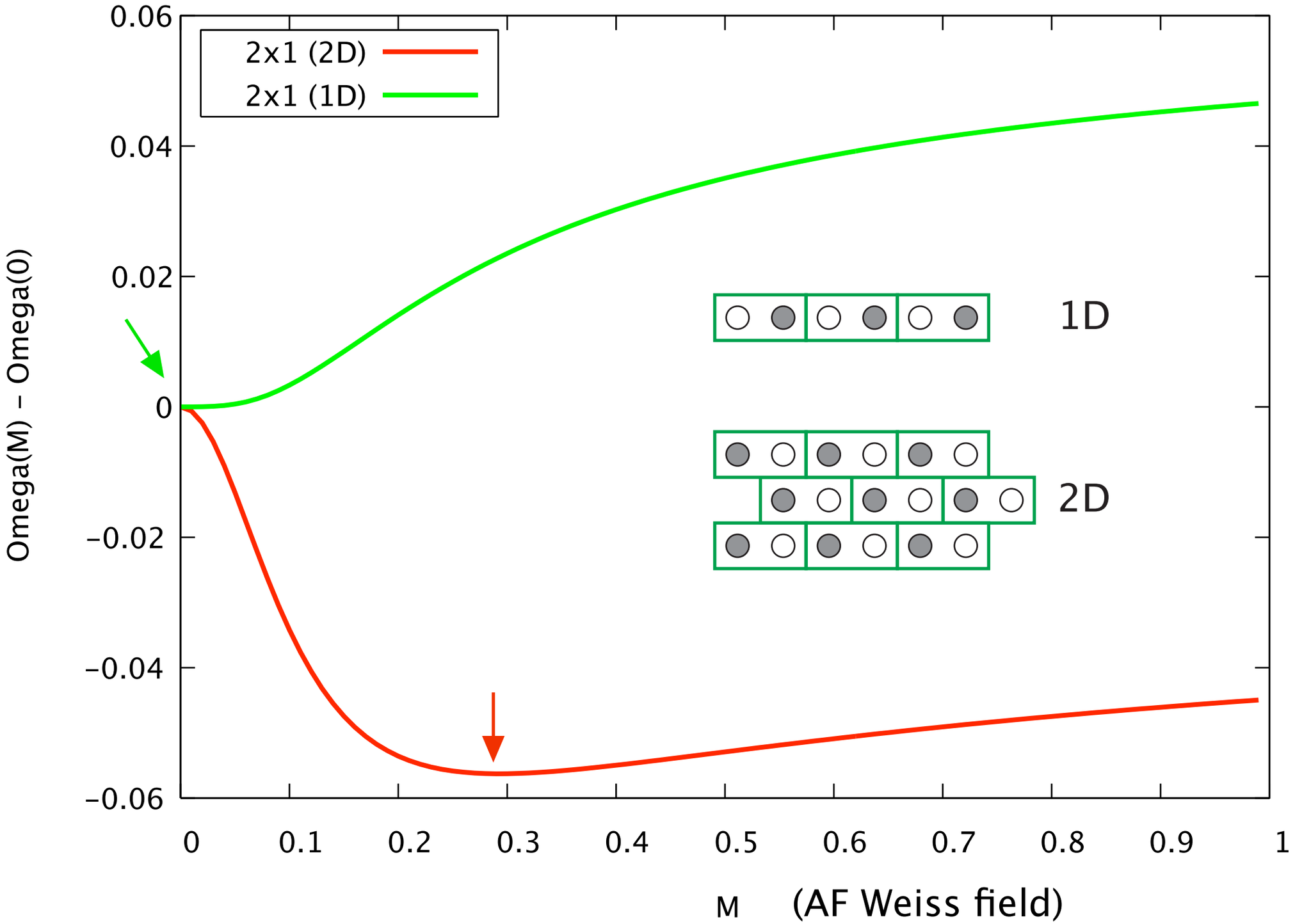
Note:

Use Gauss-Legendre integration by segments

Special orthogonal polynomials sometimes used: weight $\ln(\omega)$

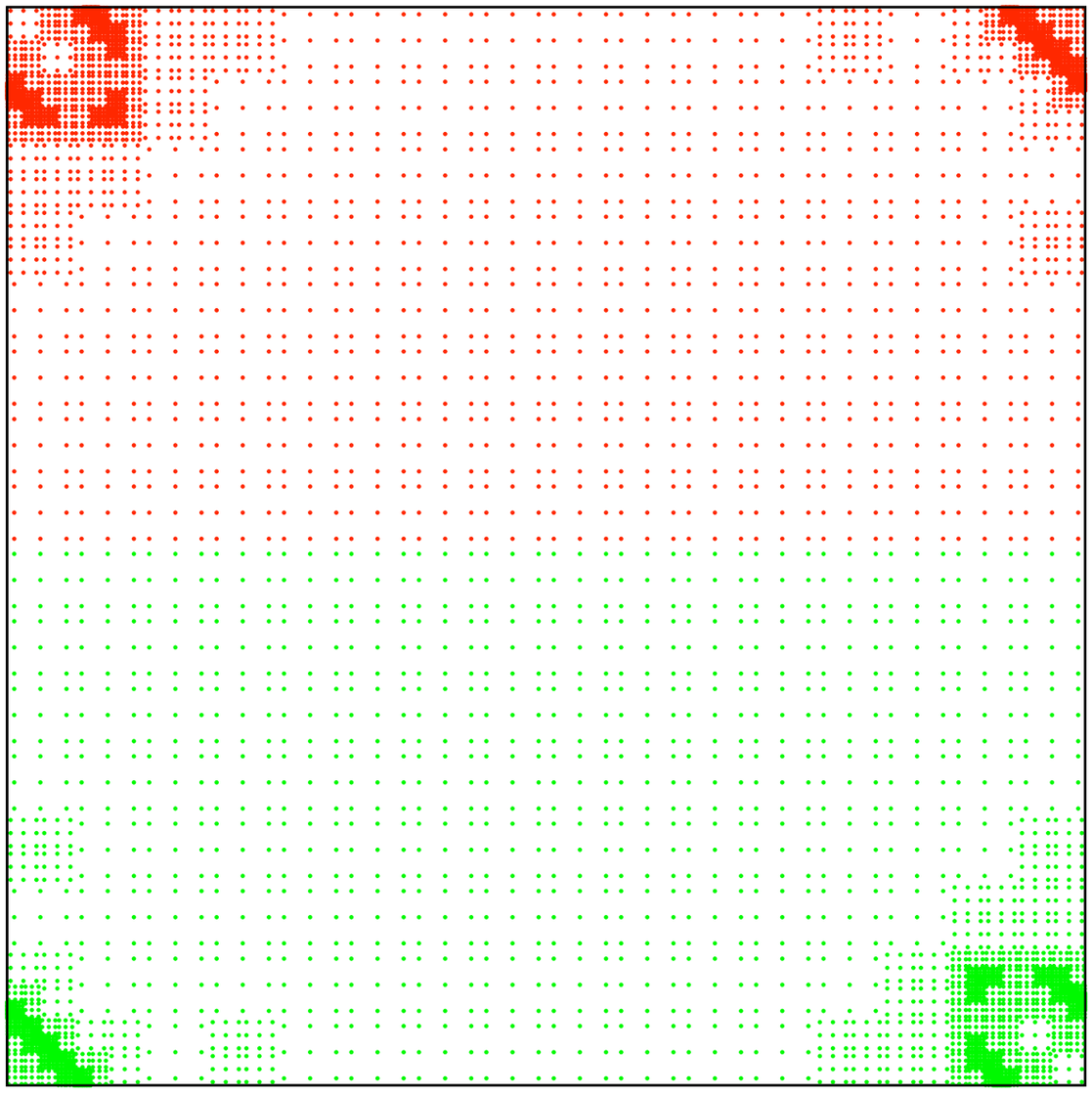
Calculation of the functional

Importance of dimensionality



Momentum integrals

- Faster to vary $\mathbf{k}$ for fixed ω than other way around
- Use a non-uniform grid if integrand is peaked



reduced Brillouin zone

3393 points

U = 4
μ = 1
t = 1
t' = -0.3
t" = 0.2
Δ = 0.4

Order parameters

Generic 1-body operator: $O = s_{\alpha\beta} c^\dagger_\alpha c_\beta$

Calculate $\langle c^\dagger_\alpha c_\beta \rangle$ from lattice Green function:

Integrate around poles of negative real axis

$$G_{\beta\alpha}(z) = \sum_n \frac{1}{z - E_n + E_0} \langle \Omega | c_\beta | n \rangle \langle n | c^\dagger_\alpha | \Omega \rangle + \frac{1}{z + E_n - E_0} \langle \Omega | c^\dagger_\alpha | n \rangle \langle n | c_\beta | \Omega \rangle$$

Nambu indices

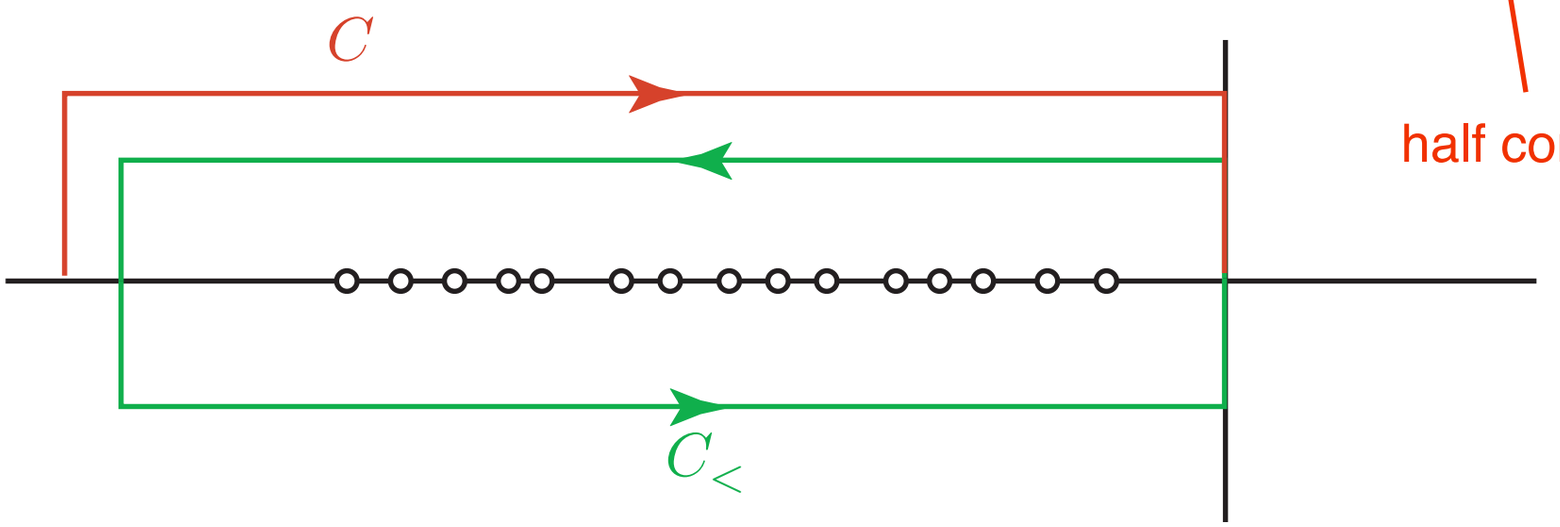
lattice GF

$$\langle O \rangle = s_{\beta\alpha} \langle c^\dagger_\beta c_\alpha \rangle = \int_{C_<} \frac{\mathrm{d}\omega}{2\pi i} \mathrm{Tr}\left[s G(z) \right] = -\mathrm{Im} \int_C \frac{\mathrm{d}\omega}{\pi} \sum_{\mathbf{K}} s^{\mu\nu}_{\mathbf{x}\mathbf{x}'}(\mathbf{K}) G^{\nu\mu}_{\mathbf{x}'\mathbf{x}}(\mathbf{K}, z)$$

site indices

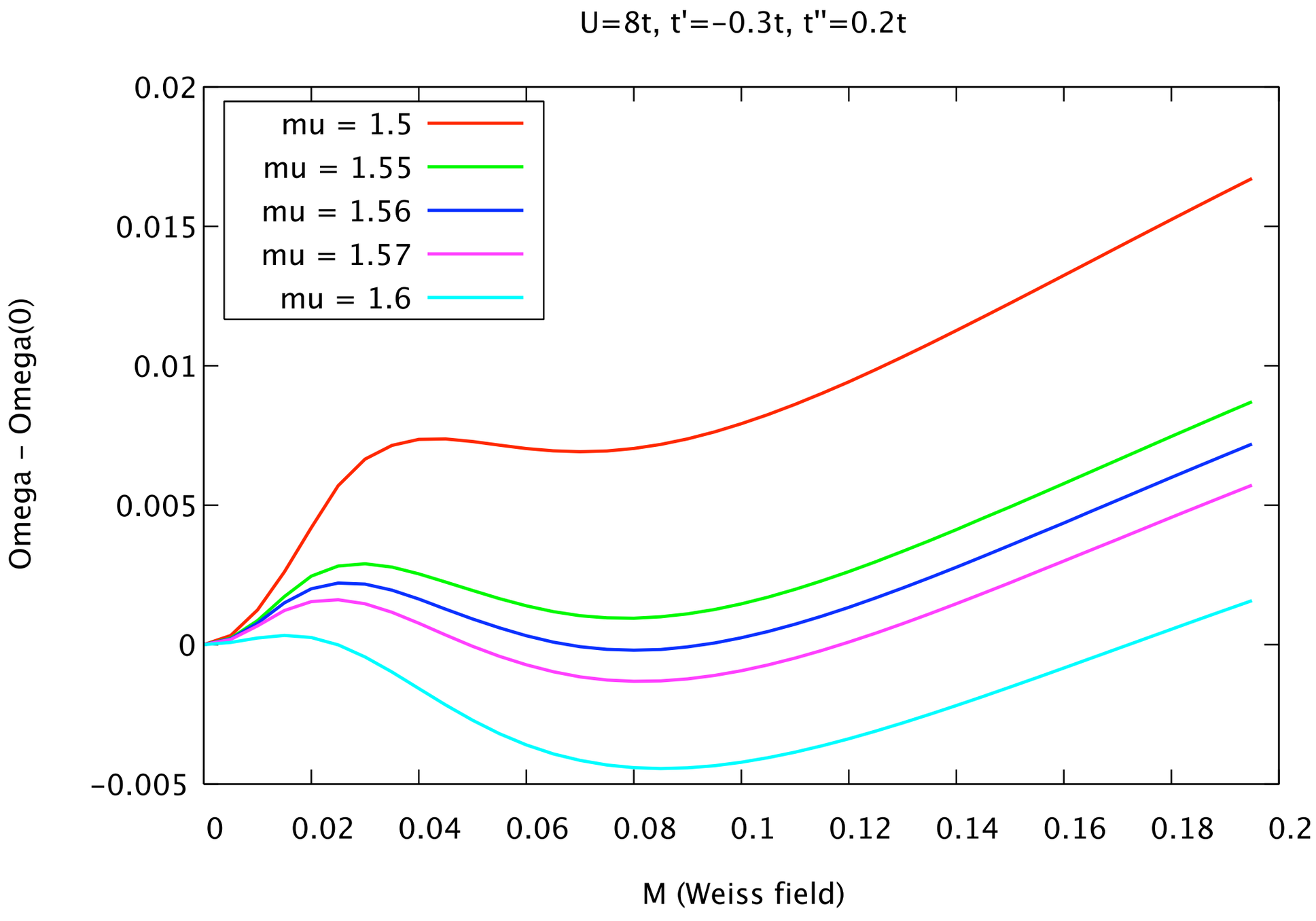
half contour

reduced BZ



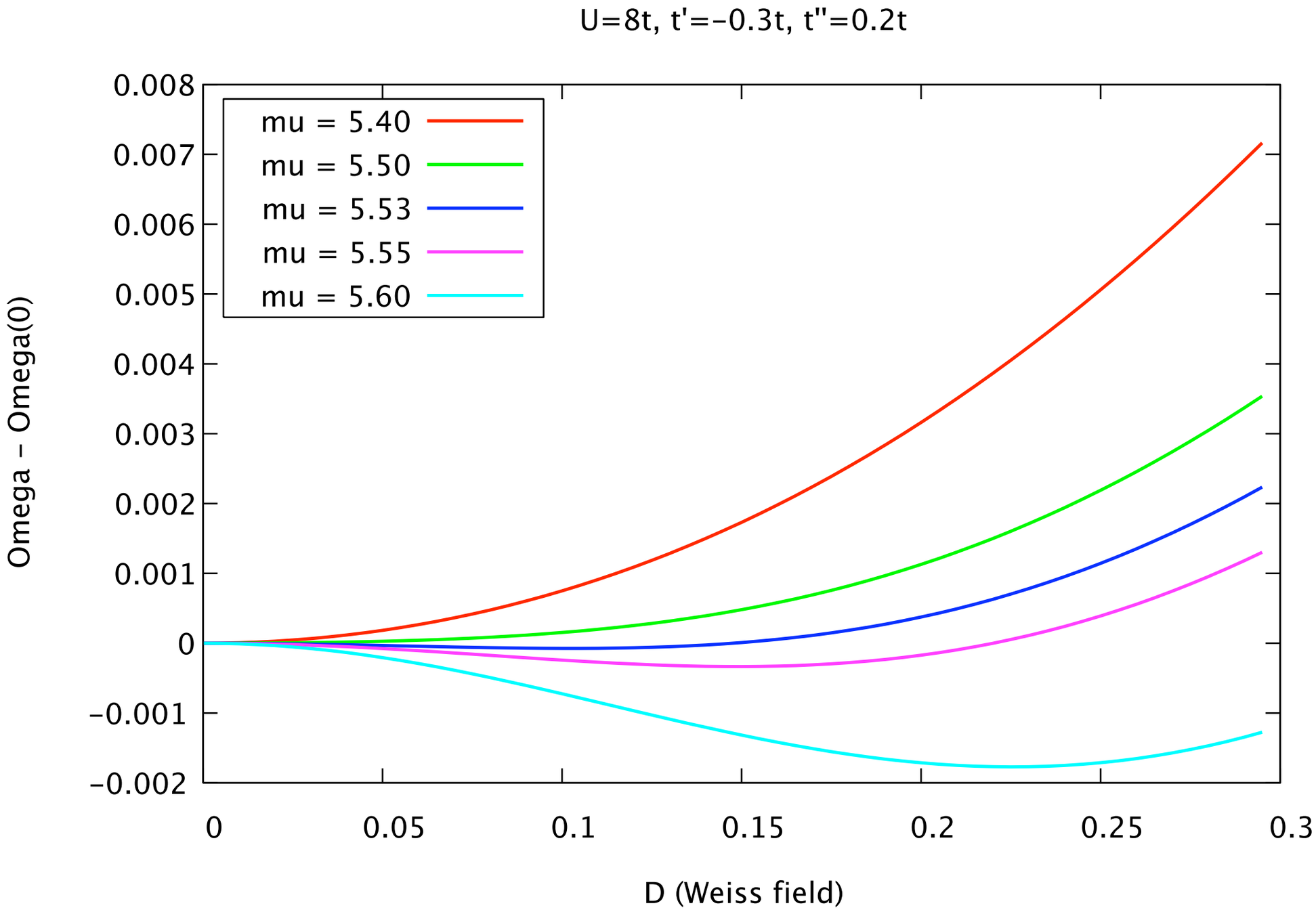
Ω vs antiferromagnetic Weiss field

example of first order transition (2x2 cluster)



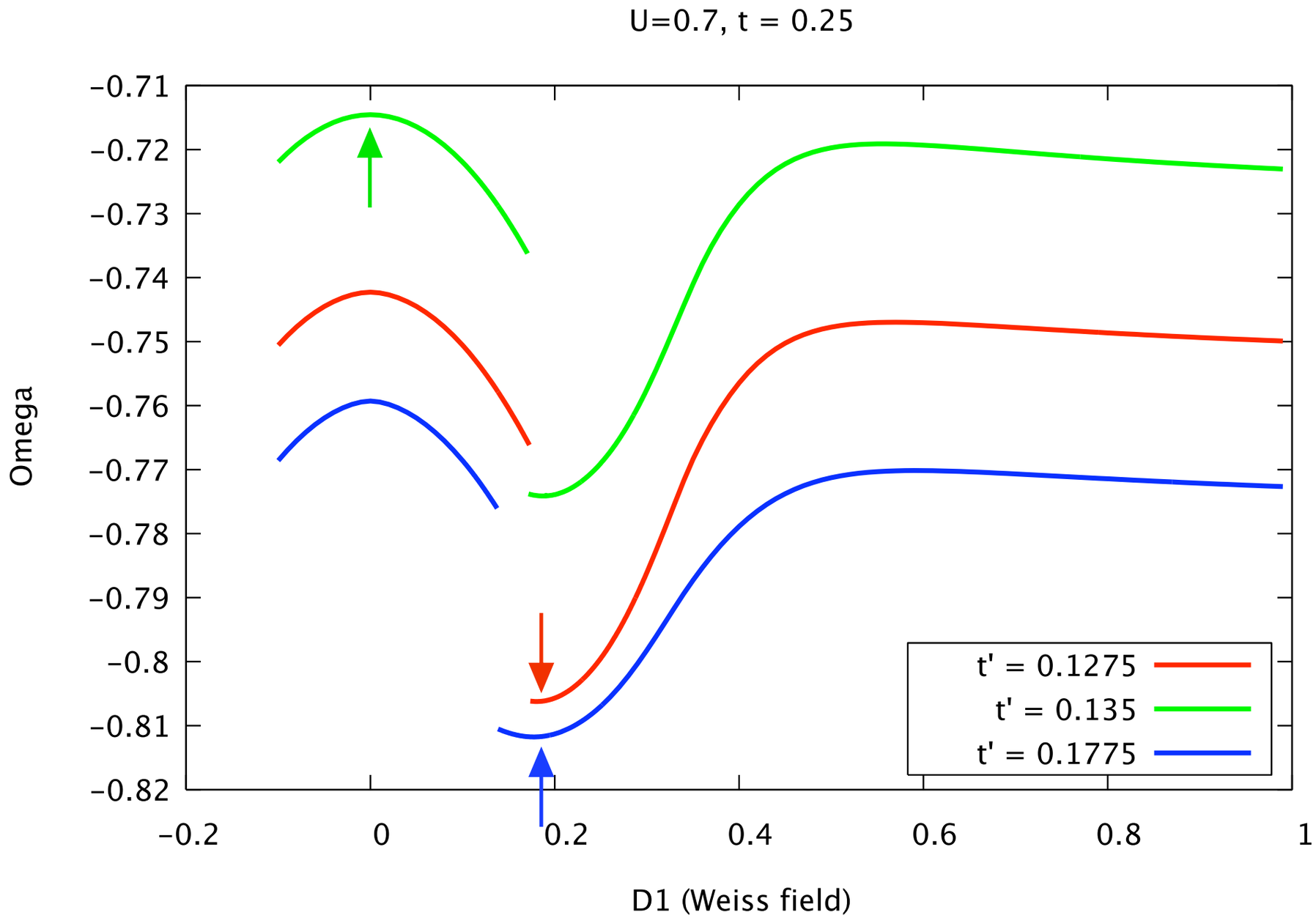
Ω vs dSC Weiss field

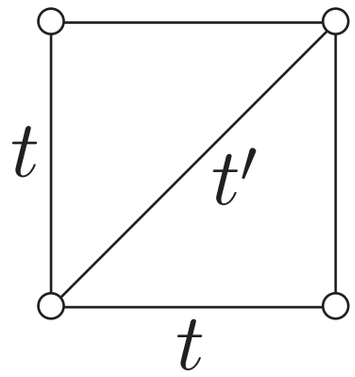
example of second order transition (2x2 cluster)



BEDT model : Ω vs d_{xy} Weiss field

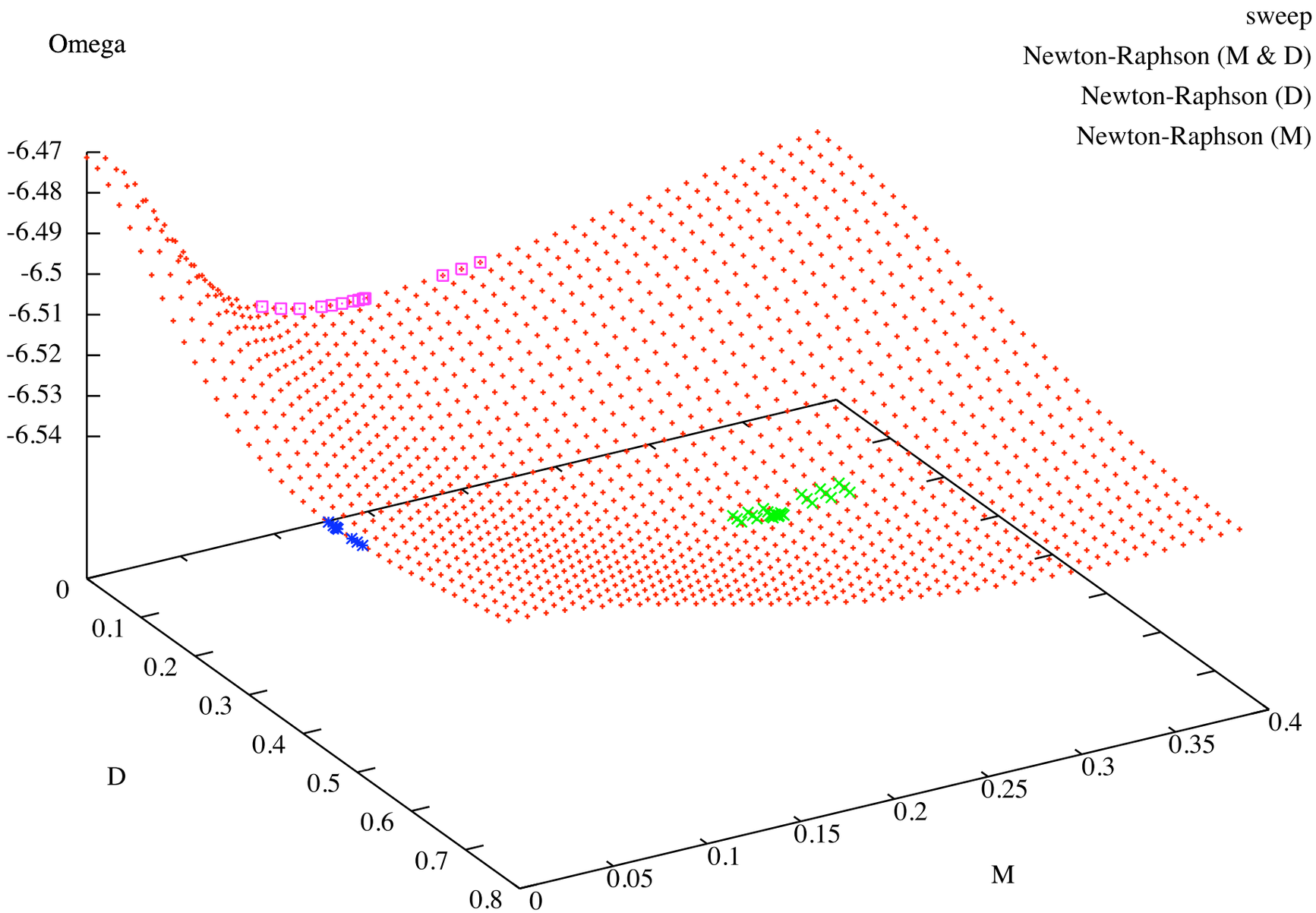
example of first order transition with discontinuity





P. Sahebsara & D. Sénéchal (in preparation).

two-parameter variation



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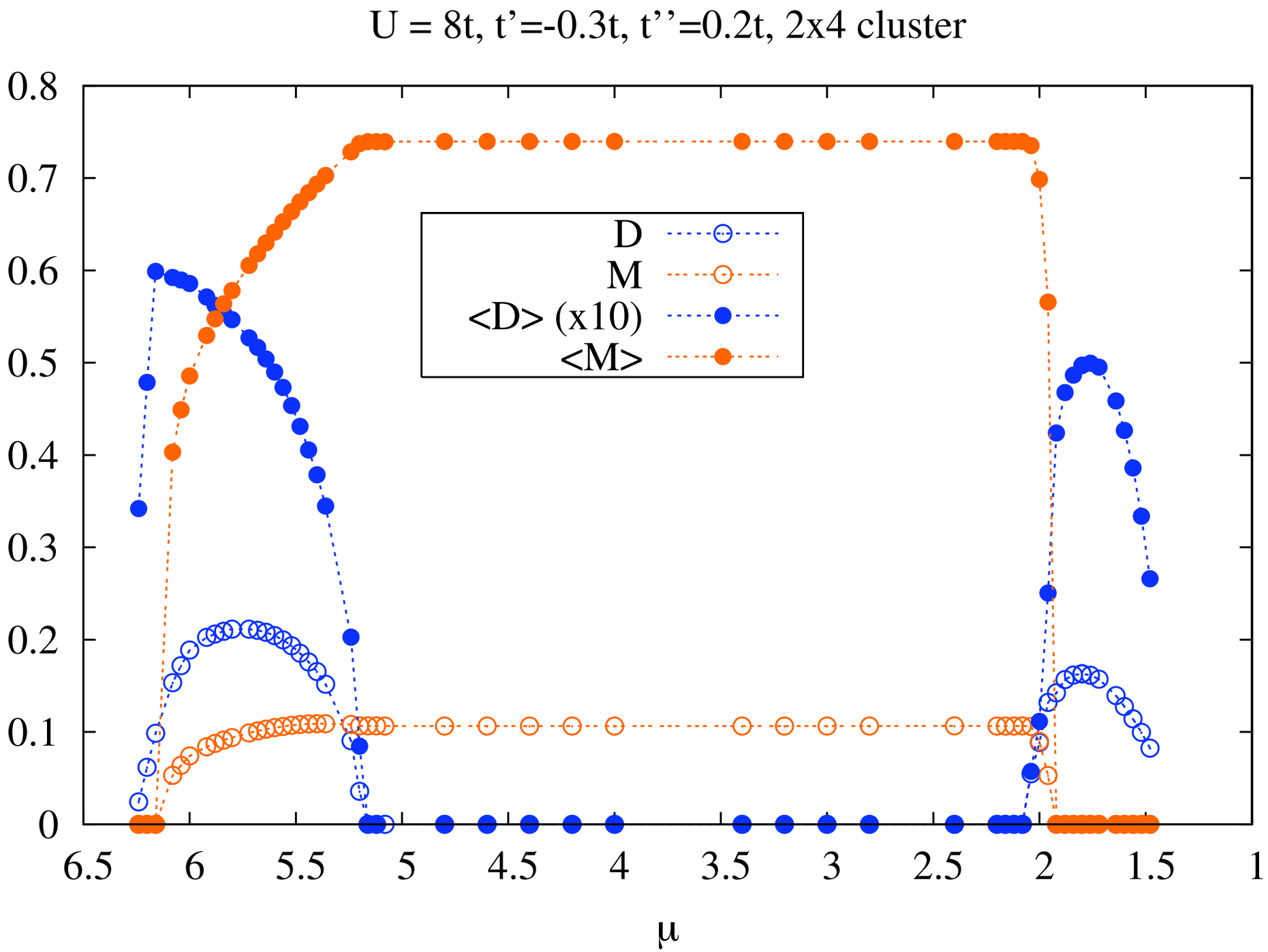
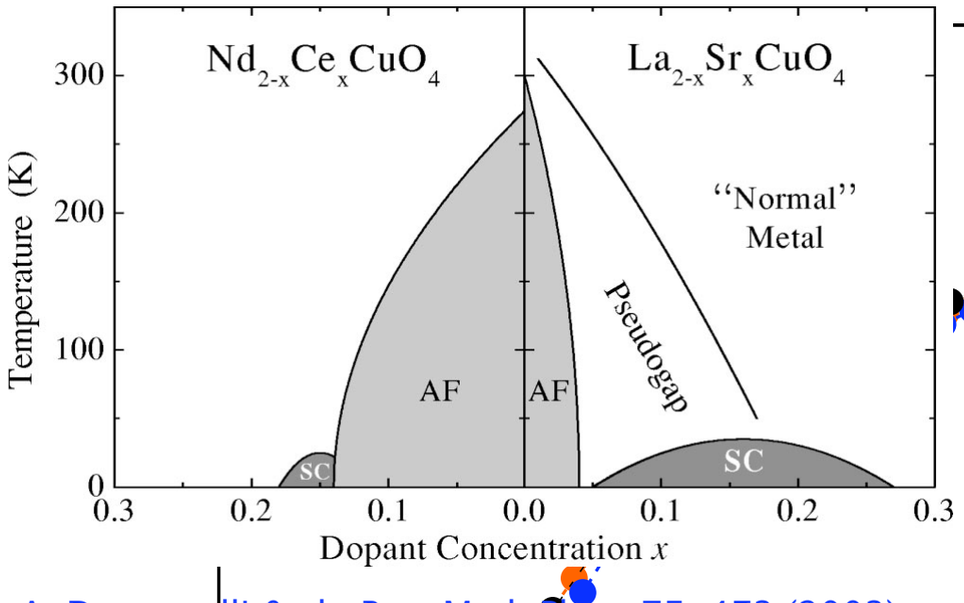
AF, d-SC Weiss fields and order parameters vs chemical potential



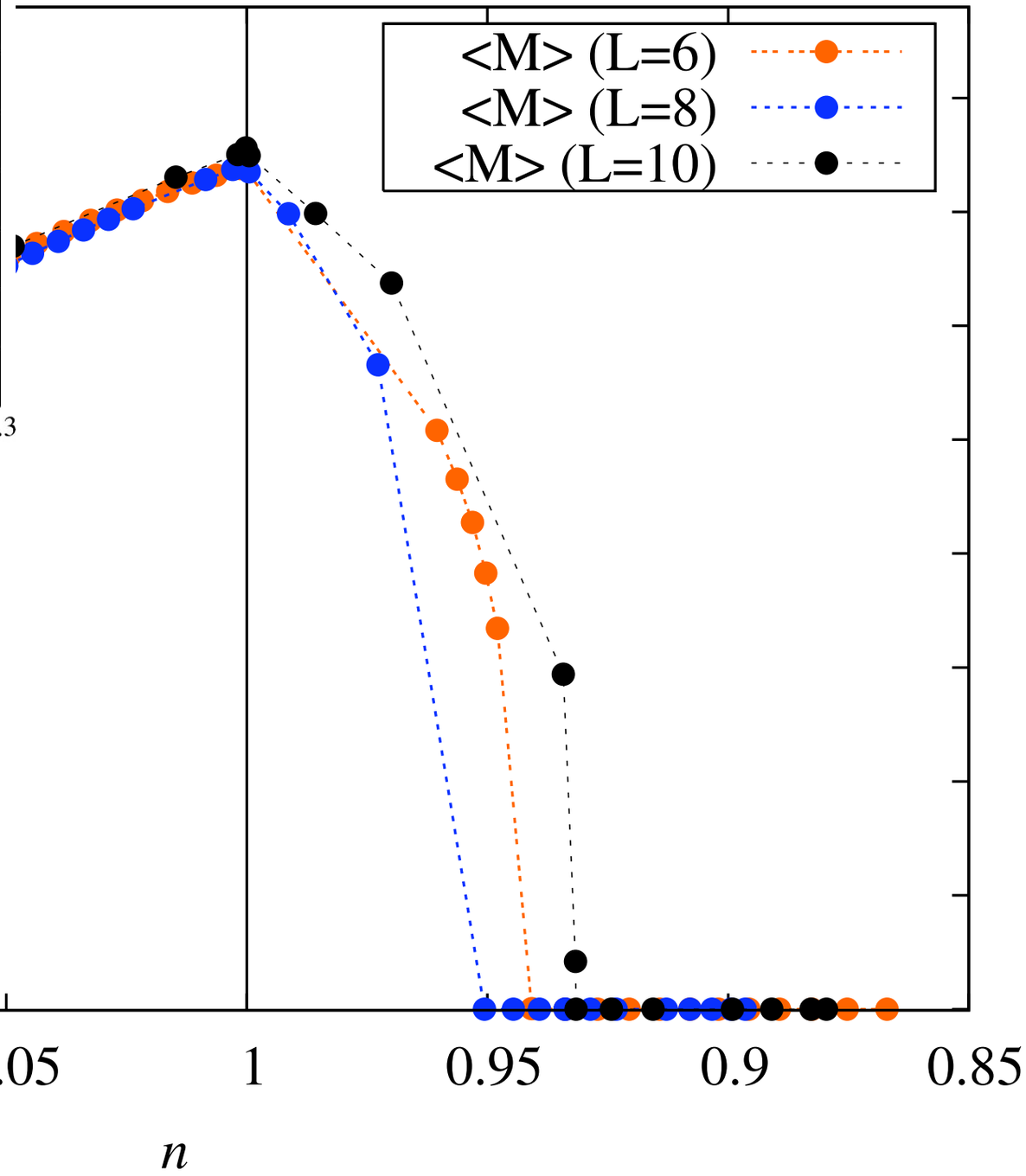
Sénéchal et al., Phys. Rev. Lett. 94, 156404 (2005).

AF order parameter

U = 8t, t'=-0.3t, t''=0.2t

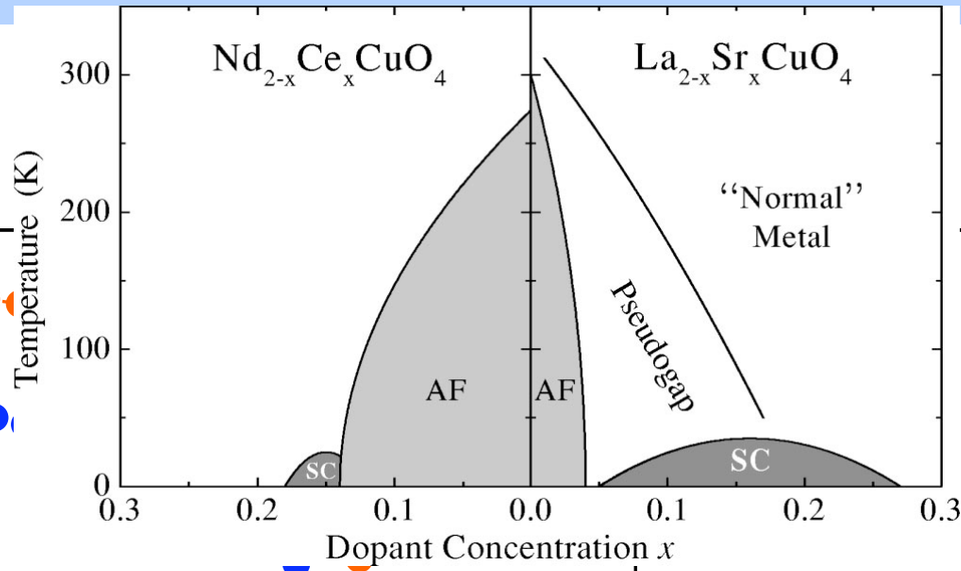


A. Damascelli & al., Rev. Mod. Phys. **75**, 473 (2003)



Sénéchal et al., Phys. Rev. Lett. 94, 156404 (2005).

d-SC order parameter

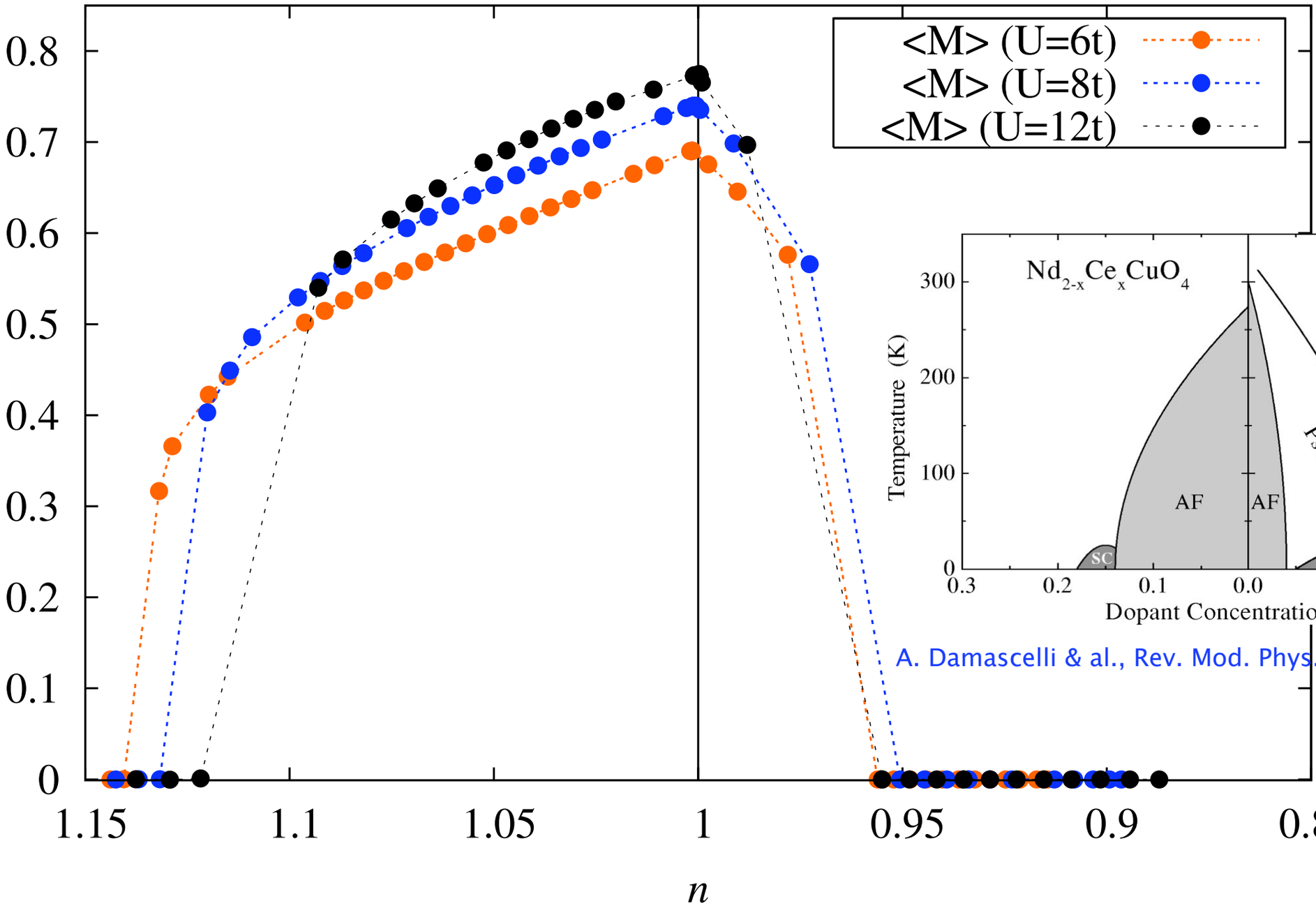


A. Damascelli & al., Rev. Mod. Phys. **75**, 473 (2003)

Sénéchal et al., Phys. Rev. Lett. 94, 156404 (2005).

AF order parameter: U = 6,8,12

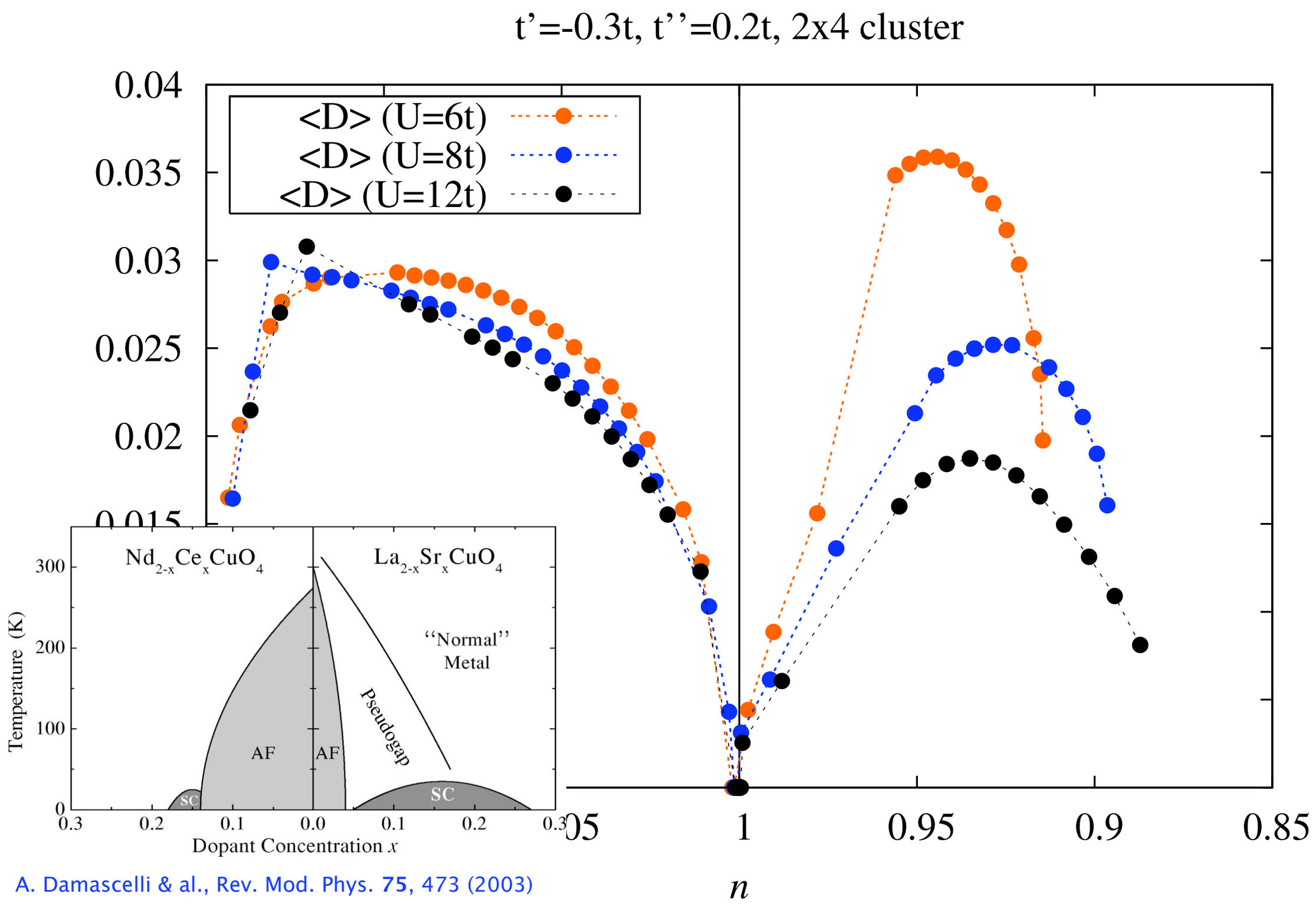
t'=-0.3t, t''=0.2t, 2x4 cluster



A. Damascelli & al., Rev. Mod. Phys. **75**, 473 (2003)

Sénéchal et al., Phys. Rev. Lett. 94, 156404 (2005).

d-SC order parameter: U=6,8,12



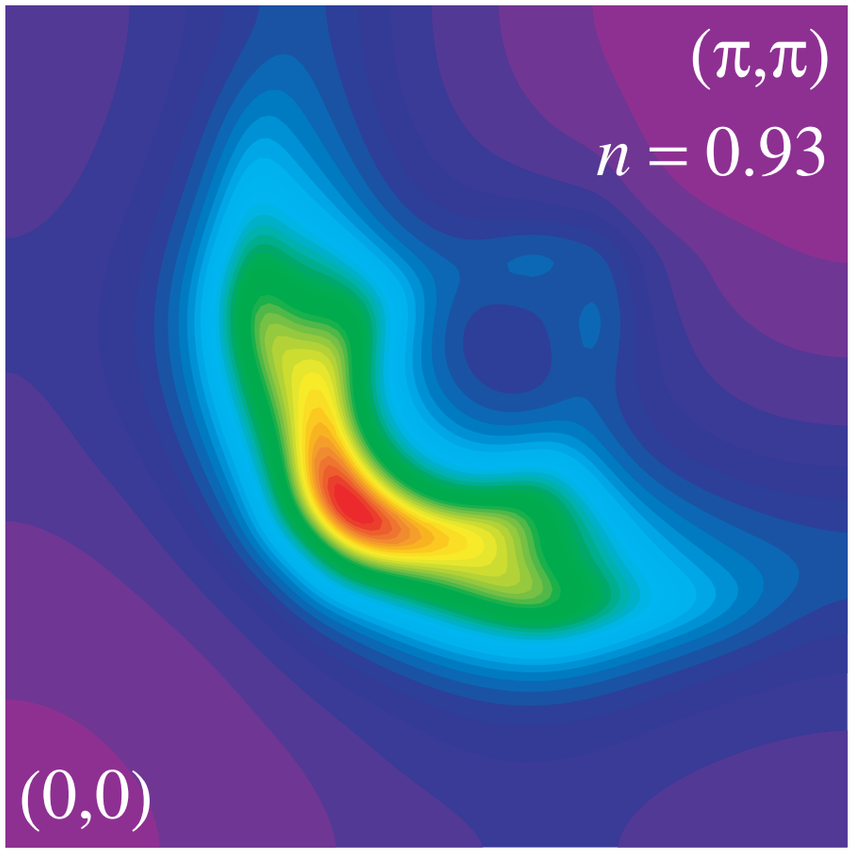
A. Damascelli & al., Rev. Mod. Phys. **75**, 473 (2003)

Sénéchal et al., Phys. Rev. Lett. 94, 156404 (2005).

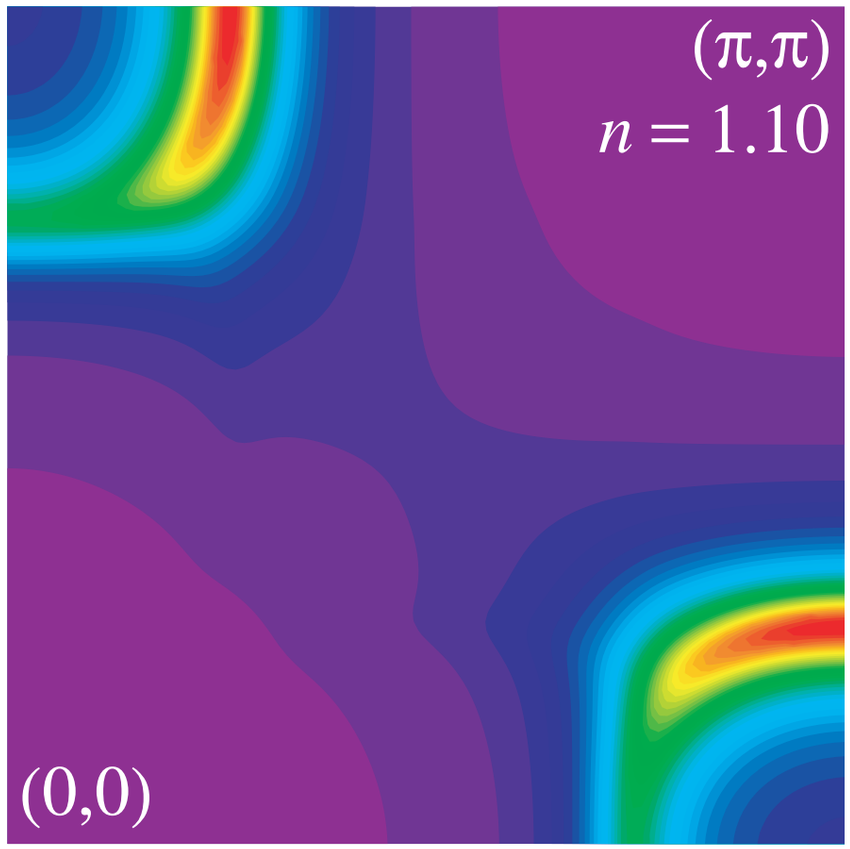
Momentum Distribution Curves

2x4 cluster, U = 8t, t'=-0.3t, t" = 0.2t

d-SC order only



d-SC + AF

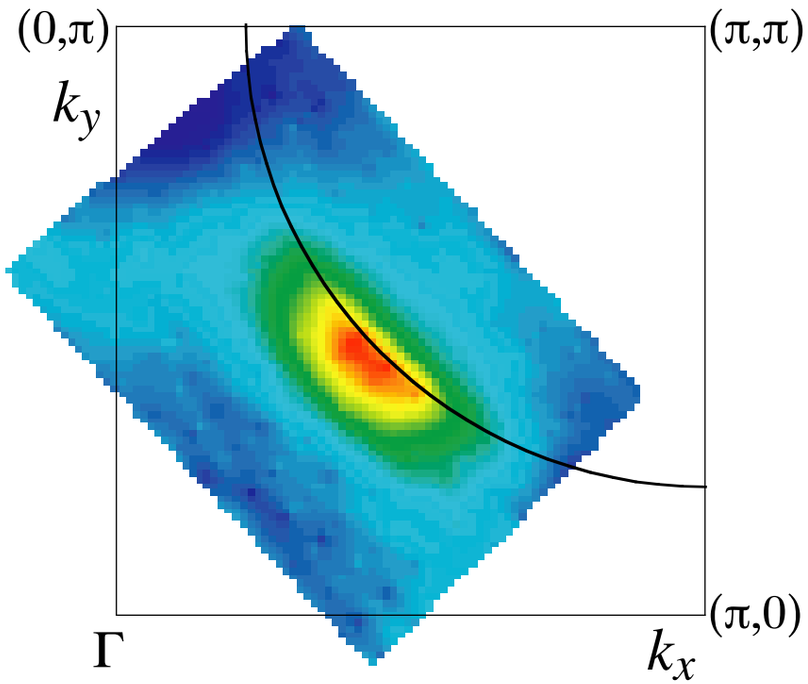


Sénéchal et al., Phys. Rev. Lett. 94, 156404 (2005).

ARPES results

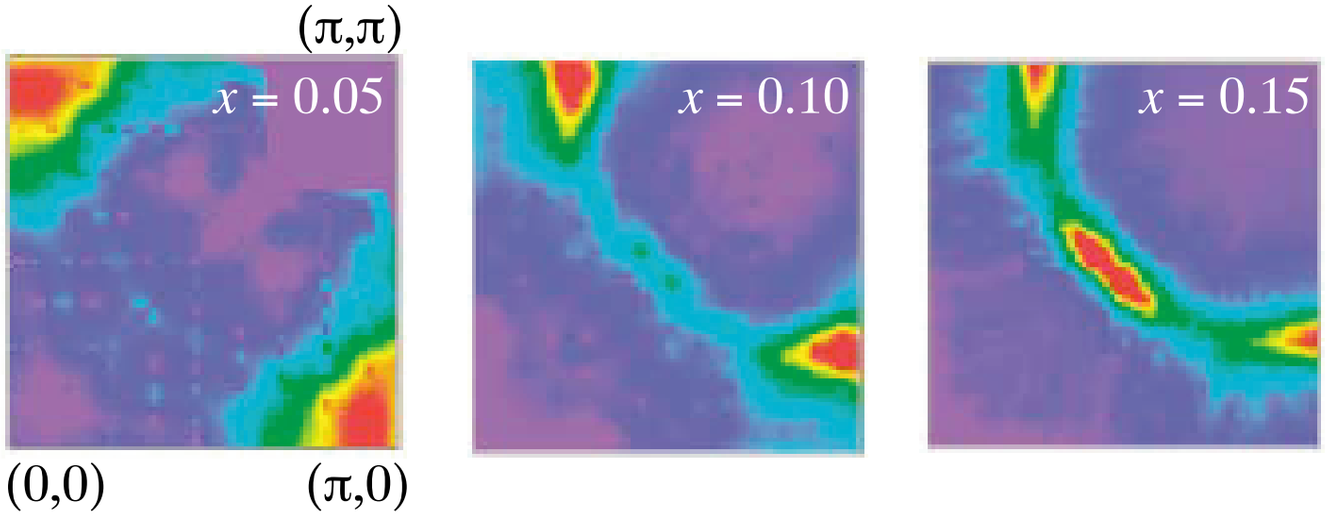
Hole-doped cuprate $Ca_{2-x}Na_xCuO_2Cl_2$

F. Ronning et al., Phys. Rev. B 67, 165101 (2003)



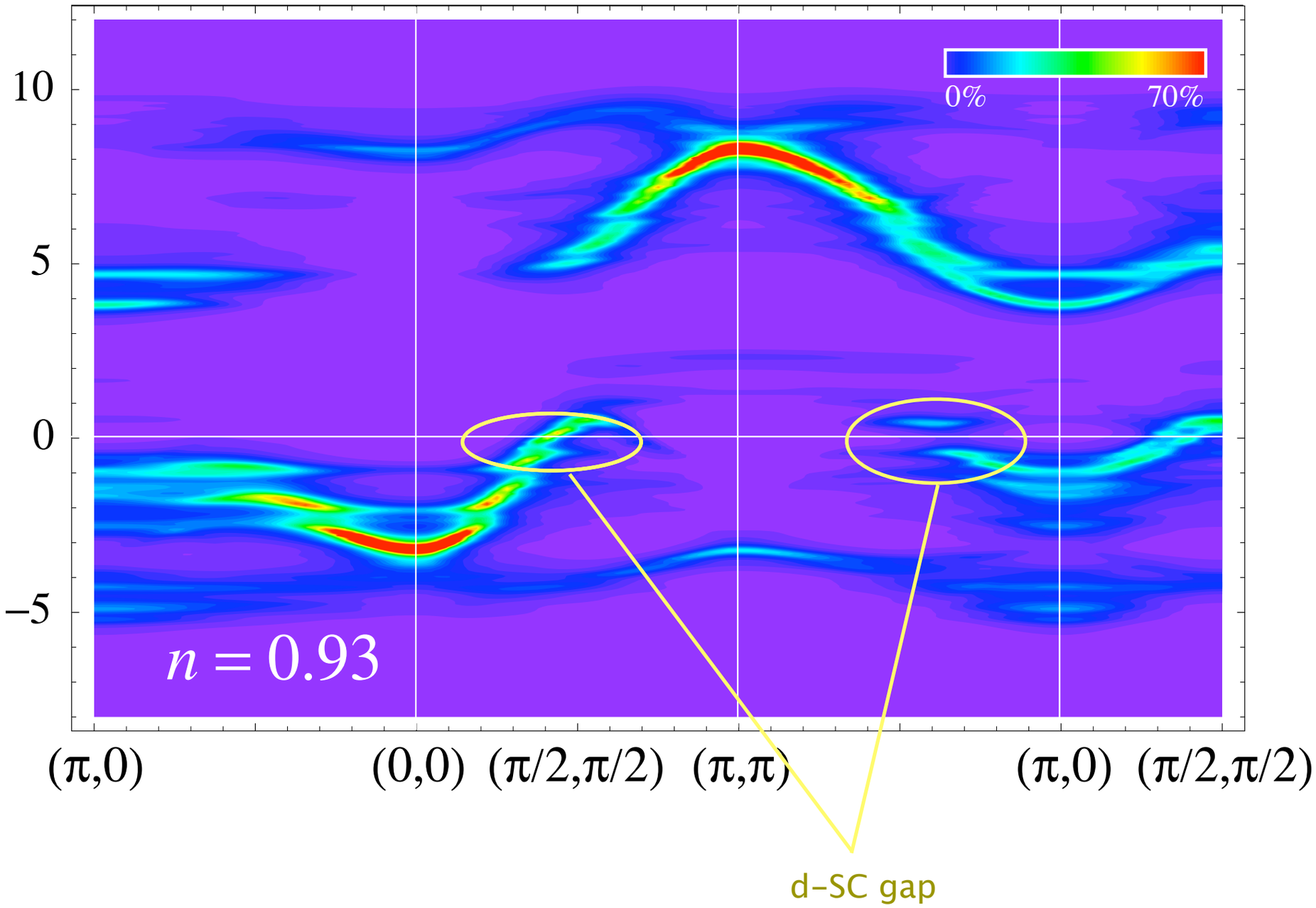
$Nd_{2-x}Ce_xCuO_4$ or NCCO (e-doped)

Armitage et al., Phys. Rev. Lett. 88, 257001 (2002)



EDCs : d-SC order

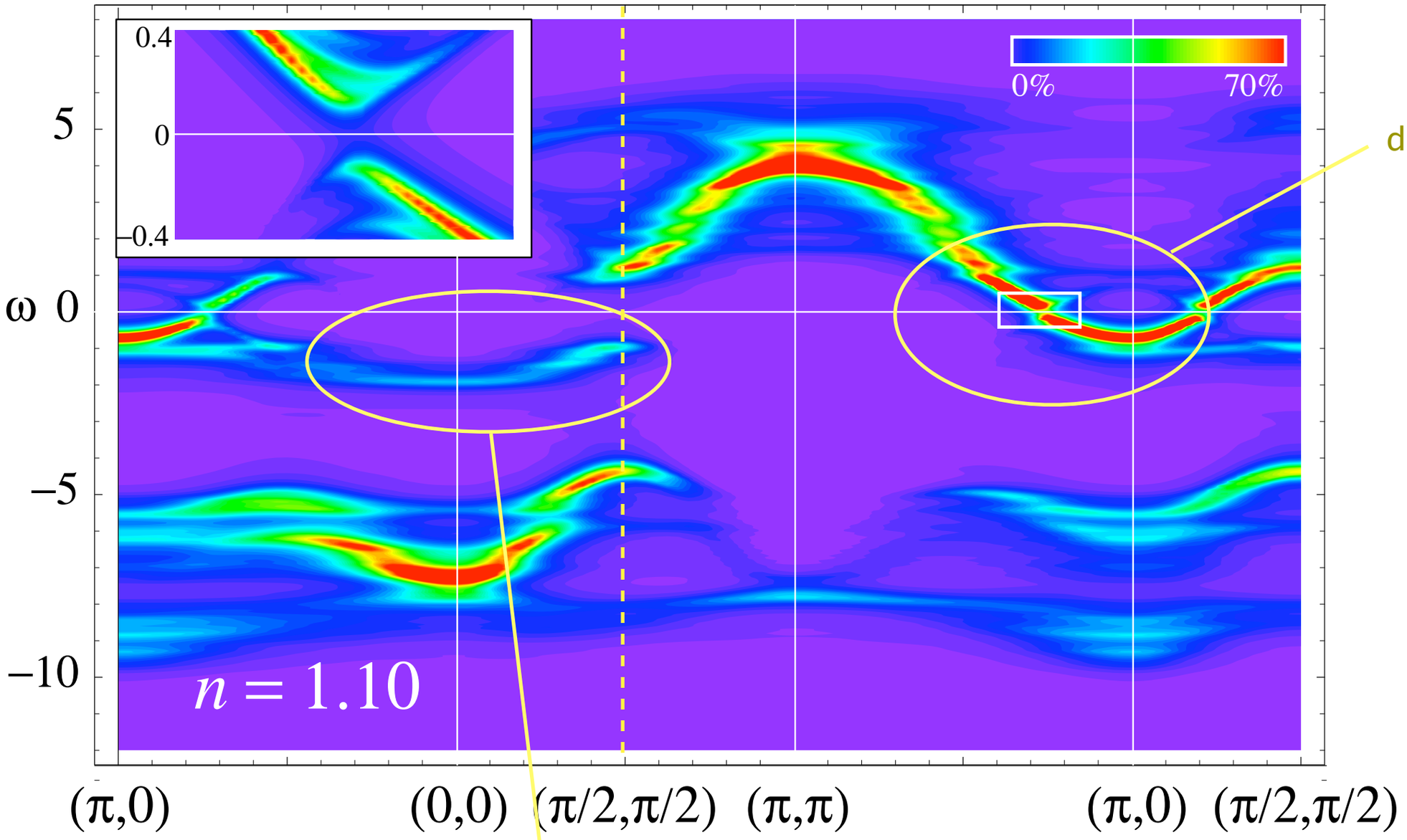
2x4 cluster, U = 8t, t'=-0.3t, t" = 0.2t, 7% h-doped



Sénéchal et al., Phys. Rev. Lett. 94, 156404 (2005).

EDCs : AF + d-SC order

2x4 cluster, U = 8t, t'=-0.3t, t" = 0.2t, 10% e-doped



Sénéchal et al., Phys. Rev. Lett. 94, 156404 (2005).

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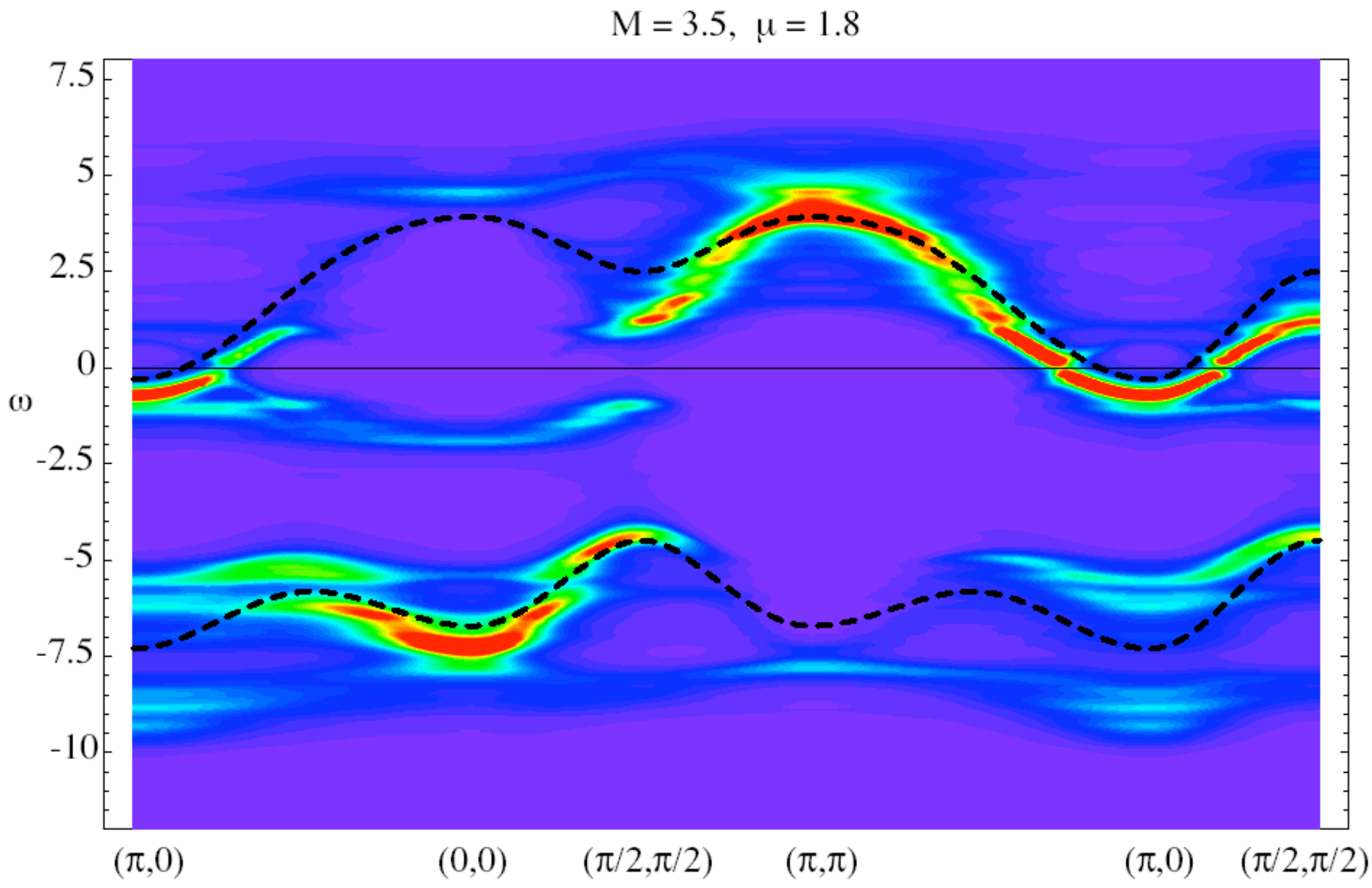
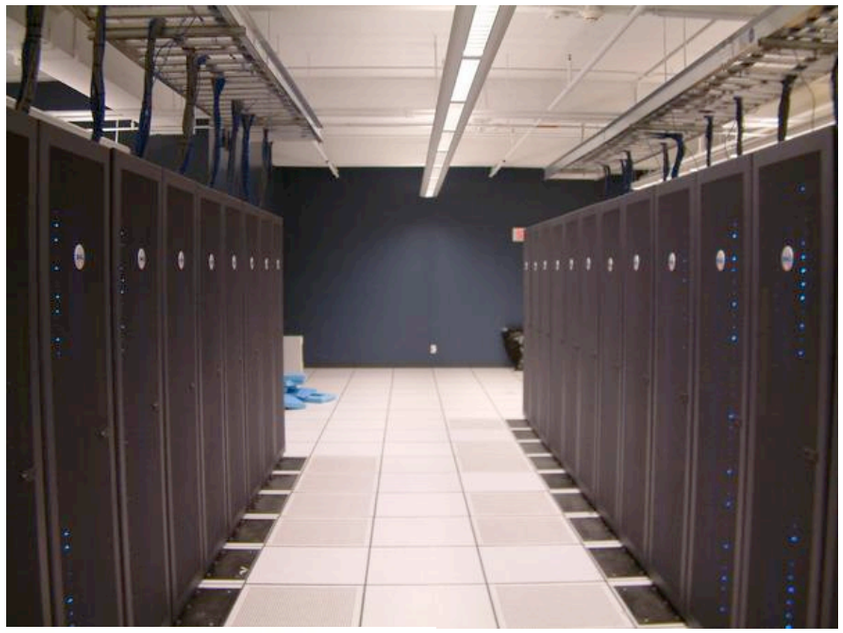


Conclusions

- General agreement with phase diagram of cuprates
  - moderate hole-doping : pure d-SC
  - small hole-doping : pure AF (shape dependent)
  - moderate electron doping : AF + d-SC
  - larger electron doping : small pure d-SC region
  - hole-doping : d-SC order parameter scales like 1/U
  - AF to d-SC transition still murky on hole-doped side (variational space too restrictive)



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THE END