Variational Cluster Approach to antiferromagnetic and superconducting phases in hole- and electron-doped cuprates

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Statement of the problem - Model

The high-temperature superconductors (HTSC) and other strongly correlated electron systems, such as heavy-fermion and a variety of transition-metal oxide systems, exhibit many ordered phases, which appear to compete and sometimes coexist.

- Antiferromagnetic (AF) order
- Superconducting (SC) order
- Coexisting AF and SC orders
- Charge- and Spin-"stripe" phases

Description on a microscopic level:

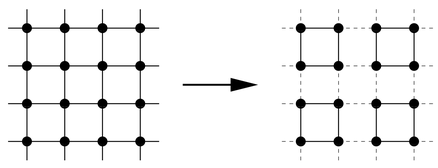
Single-band Hubbard model:

$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow})$$

- Hopping integrals:
  - n.n. hopping $t = 1$ (unit of energy)
  - n.n.n. hopping $t' = -0.3t$
- Hubbard interaction $U = 8t$
- Chemical potential μ: Filling control

Method - Variational Cluster Approach

First step: Tiling of the lattice into clusters of finite size:



Finite clusters ≡ Reference systems for SFA

The main property of the SFA/VCA method is the Grand potential:

$$\Omega(\mathbf{\Delta}) = \Omega'(\mathbf{\Delta}) + T \sum_{\omega_n, \mathbf{Q}} \mathrm{tr}\, \ln \frac{-\mathbf{1}}{\mathbf{G}^{(0)}_{\mathbf{Q}}(i\omega_n)^{-1} - \mathbf{\Sigma}(\mathbf{\Delta}, i\omega_n)} - LT \sum_{\omega_n} \mathrm{tr}\, \ln(-\mathbf{G}'(\mathbf{\Delta}, i\omega_n)).$$

Exact quantities (reference system): $\Omega'(\mathbf{\Delta})$, $\mathbf{\Sigma}(\mathbf{\Delta}, i\omega_n)$, and $\mathbf{G}'(\mathbf{\Delta}, i\omega_n)$

Variational parameters $\mathbf{\Delta}$:
Staggered magnetic field, d-wave pairing field, onsite potential $\Delta\mu'$

Variational principle:

Physical solution $G \Leftrightarrow \frac{\partial \Omega}{\partial \Delta_i} = 0$

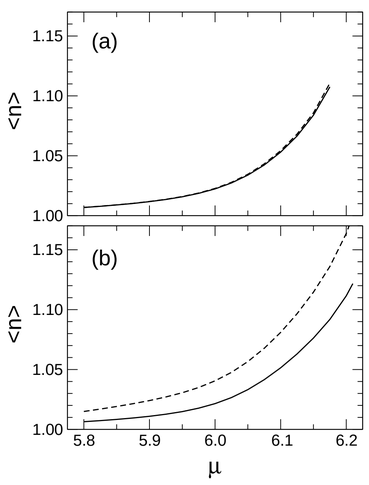
Thermodynamic consistent particle density

Variational parameter $\Delta\mu'$ ensures thermodynamic consistent density

$$-\frac{\partial \Omega}{\partial \mu} = \sum_{i\sigma} \int f(\omega) A_{ii\sigma}(\omega) \mathrm{d}\omega$$

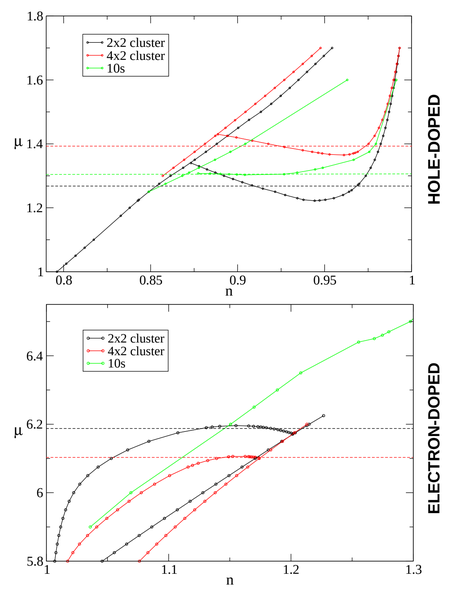
with optimization of $\Delta\mu'$:

without optimization of $\Delta\mu'$:



Competing AF and SC orders

Small reference systems show tendency to phase separation.



Chemical potential μ as function of the electron density n.
Dotted lines ≡ critical μ. Maxwell construction for phase separation.

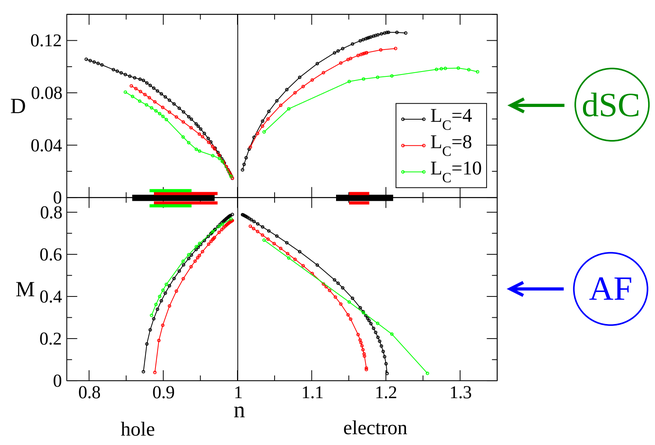
Order parameters

Antiferromagnetic order parameter:

$$M = -\frac{1}{\pi} \mathrm{Im} \frac{1}{L} \sum_{\mathbf{k}} \int \mathrm{d}\omega \sum_\sigma (-1)^\sigma G_\sigma(\mathbf{k}, \mathbf{k}+\mathbf{Q}, \omega), \quad \mathbf{Q} = (\pi, \pi)$$

Superconducting order parameter:

$$D = -\frac{1}{\pi} \mathrm{Im} \frac{1}{L} \sum_{\mathbf{k}} \int \mathrm{d}\omega\, g(\mathbf{k}) F(\mathbf{k}, \mathbf{k}, \omega), \quad g(\mathbf{k}) = \cos(k_x) - \cos(k_y)$$



Bars mark the regions of Phase Separation.
Order parameters show coexisting SC+AF phases!
AF regime is enhanced on the electron-doped side (as in experiments).

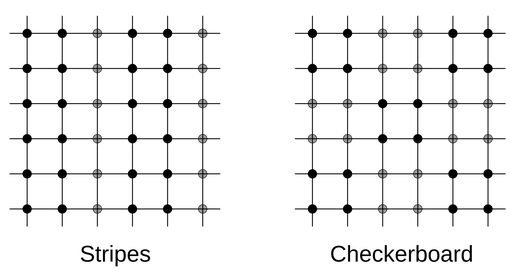
Is it phase separation?

Small reference systems (2x2, 4x2) show Phase Separation.

BUT: Phase separation energy decreases with cluster size!
Longer-range Coulomb interactions neglected!

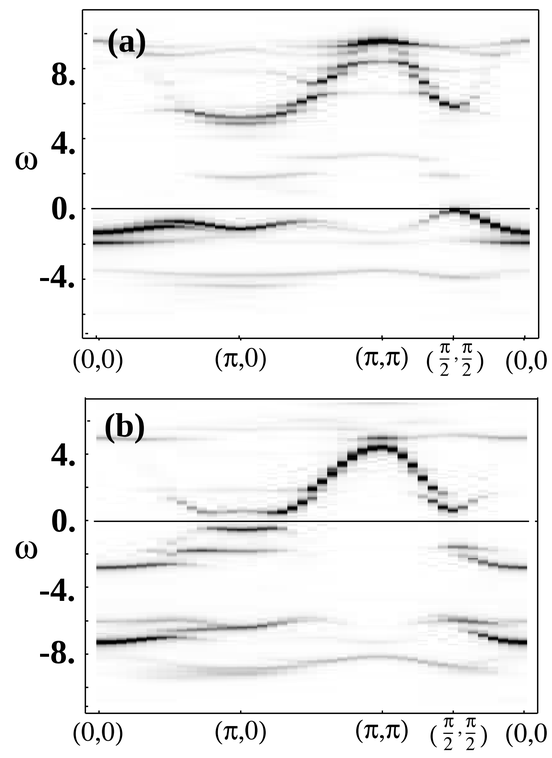
Alternative scenario: Microscopic inhomogenities!

Possible microscopic order patterns:



Can be simulated by additional variational parameter (to be done...)

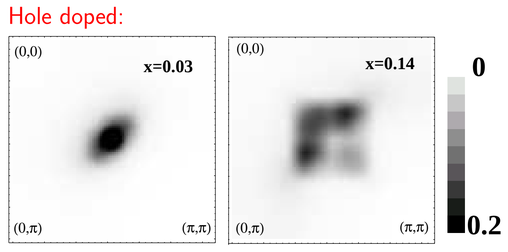
Spectral functions



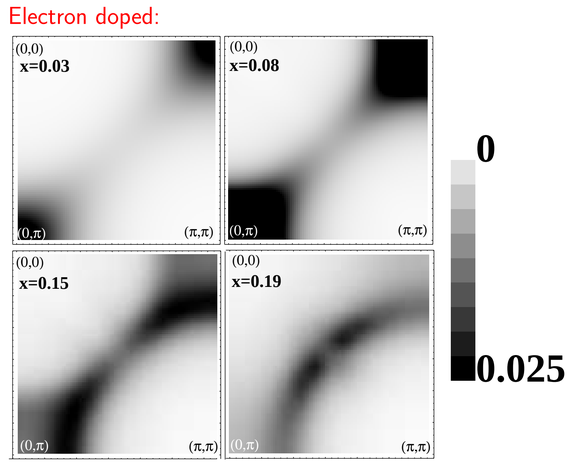
Spectral functions just before the transition to a non-magnetic state:
Upper panel: Hole doping, $x \approx 0.03$
Lower panel: Electron doping, $x \approx 0.13$

Fermi surfaces

Hole doped:



Electron doped:



Hole doped:

Hole pockets around $(\pi/2, \pi/2) \longrightarrow$ FS around (π, π).

Electron doped:

Pockets around $(\pi, 0) \longrightarrow$ FS around (π, π).

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References

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[3] M. Potthoff, M. Aichhorn, and C. Dahnken, Phys. Rev. Lett. **91**, 206402 (2003).