Quantum Cluster Methods for Strongly Correlated Electron Systems:

Variational Approach

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Advanced School of Recent Progress in
Condensed Matter Physics and Strongly Correlated Systems

IPM

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UNIVERSITÉ DE SHERBROOKE

Réseau québécois de calcul de haute performance

NSERC CRSNG

Menu

Part I :

Correlated Electron Systems

Part II :

Quantum Cluster Methods

Part III:

Variational Approach

Summary

Part I :

- Lanczos algorithm (or Band Lanczos) is able to diagonalize the Hamiltonian Matrix for a small systems, and calculates the Green function

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Part II :

- CPT :
  - The lattice is tiled by small identical clusters
  - It is able to calculate the Green function of the lattice, by solving the problem for small clusters
- SFA :
  - The grand potential can be written as a functional of the self-energy Σ
  - $F[\Sigma]$ is universal $\rightarrow$ $\Omega_t[\Sigma] = \Omega' - \mathrm{Tr}\,\ln(1 - \mathsf{V}\mathsf{G}')$
  - For a set of physical variable, grand potential is the saddle point in Ω-space. Now it is a function of the physical variables.

Part III

The Variational Cluster Approximation

Motivation

- CPT cannot describe broken symmetry states, because of the finite cluster size
- Idea : add a Weiss field term to the cluster Hamiltonian *H'*, e.g., for antiferromagnetism:

$$H'_M = M \sum_a \mathrm{e}^{i\mathbf{Q}\cdot\mathbf{r}_a}(n_{a\uparrow} - n_{a\downarrow})$$

- This term favors AF order, but does not appear in *H*, and must be subtracted from *V*
- SFA is the principle to set the value of *M* .

VCA : Basic Idea

- Set up a superlattice of clusters
- Choose a set of variational parameters,

  e.g. Weiss fields for broken symmetries
- Set up the calculation of the Potthoff functional:

$$\Omega_t[\Sigma] = \Omega' - \frac{TL}{N} \sum_{\omega} \sum_{\tilde{\mathbf{k}}} \ln \det \left[1 - \mathsf{V}(\tilde{\mathbf{k}}) \mathsf{G}'(\tilde{\mathbf{k}}, \omega) \right]$$

- Use an optimization method to find the stationary points
- Adopt the cluster self-energy associated with the stationary point, and use it for the lattice

Variational Cluster Approximation

$$\left.\frac{\delta\Omega[\Sigma]}{\delta\Sigma}\right|_{\Sigma_{physical}} = 0$$

- Therefore, $\Omega[\Sigma]$ can be written as the direct function of the physical variables h:

$$\Sigma = \Sigma(h)$$

$$\Omega = \Omega[\Sigma(h)] = \Omega(h)$$

Variational Cluster Approximation

$$\Omega = \Omega(h)$$

- Best values of hopping and Weiss fields determined by a rigorous variational principle:

$$\frac{\delta\Omega}{\delta h} = 0$$

where $\Omega = (E - \mu N)$ is the grand potential at the physical solution.

Variational Cluster Approximation

- We add a Weiss field term to the cluster Hamiltonian *H'*
- This term favors AF order, but does not appear in *H*, and must be subtracted from *V*

Neel order

$$H'_{AF} = M\sum_i (-1)^{\sigma} e^{i\mathbf{Q}.\mathbf{r}_i} n_{i\sigma} \quad , \quad \mathbf{Q} = (\pi,\pi)$$

d-wave SC

$$H'_{SC} = \sum_{\langle i,j\rangle} \left(\Delta_{ij} c_{i\uparrow} c_{j\downarrow} + \text{h.c.}\right)$$

Filling

$$H'_{\mu} = -\mu \sum_{i\sigma} n_{i\sigma}$$

Spiral order

$$H'_{120^\circ} = h\left\{\sum_{i\in A} e_A.S_i + \sum_{i\in B} e_B.S_i + \sum_{i\in C} e_C.S_i\right\}$$

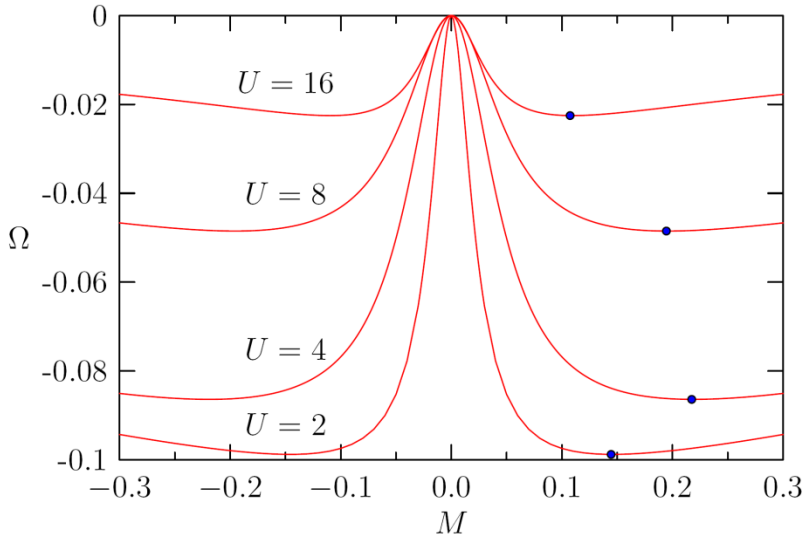
$$\frac{\delta\Omega}{\delta M} = 0 \quad , \quad \frac{\delta\Omega}{\delta\Delta_{ij}} = 0$$

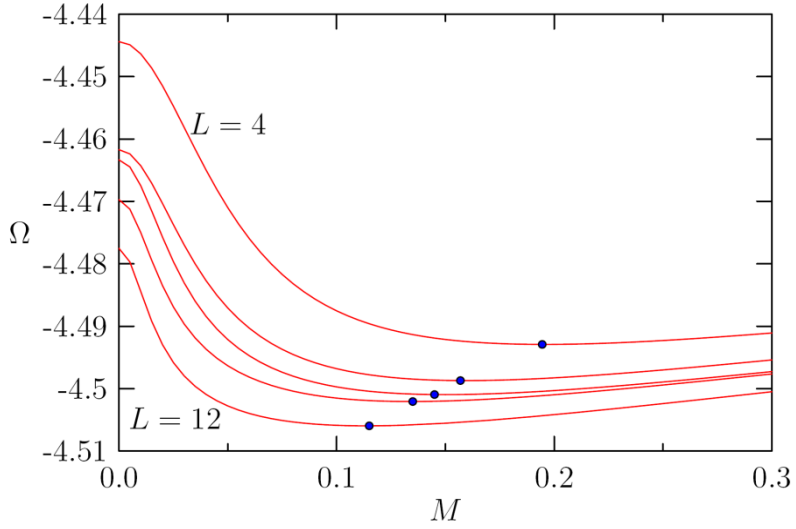
VCA : Néel Antiferromagnetism

The AF Weiss field :

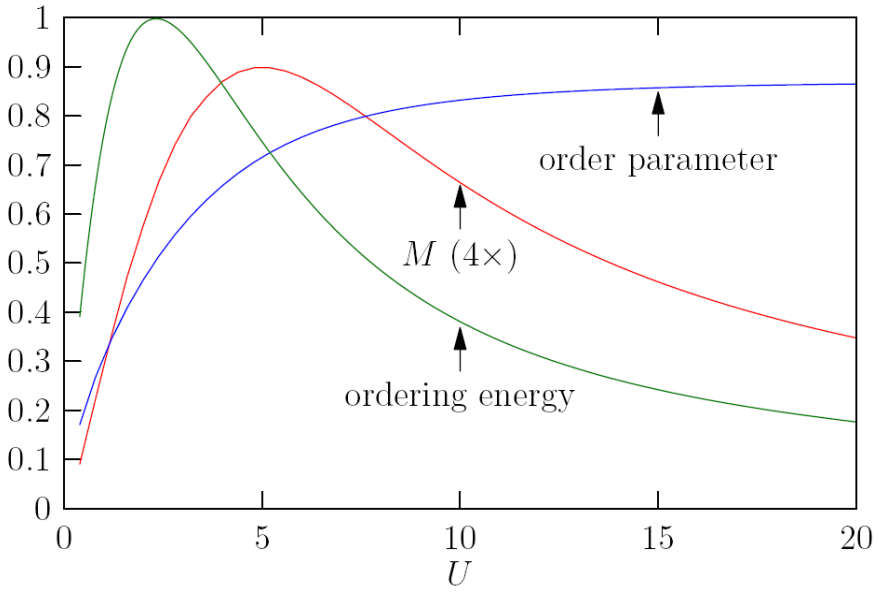
$$H'_M = M \sum_a \mathrm{e}^{i\mathbf{Q}\cdot\mathbf{r}_a}(n_{a\uparrow} - n_{a\downarrow})$$

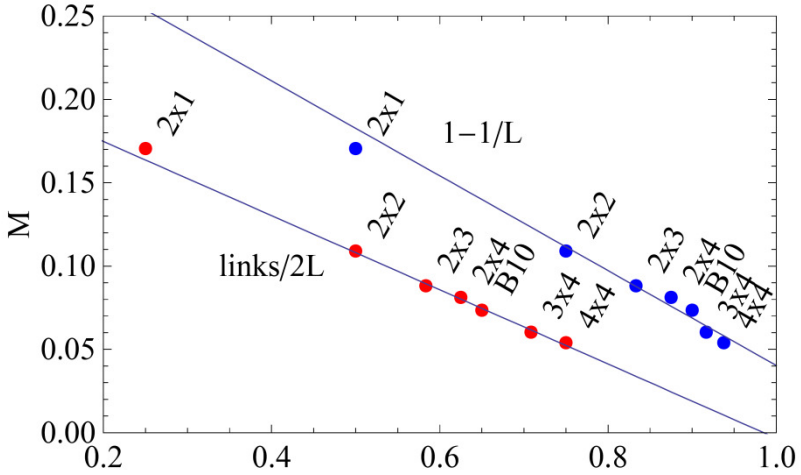
Ω for the half-filled, square lattice Hubbard model:

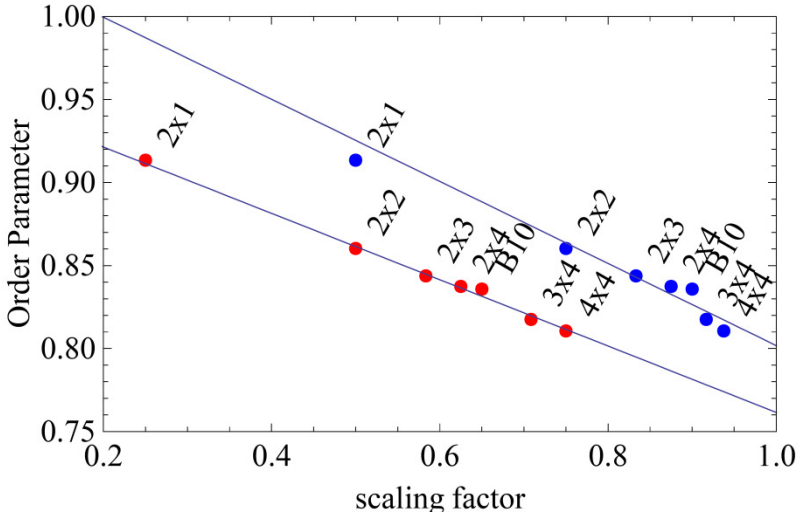




VCA : scaling factor







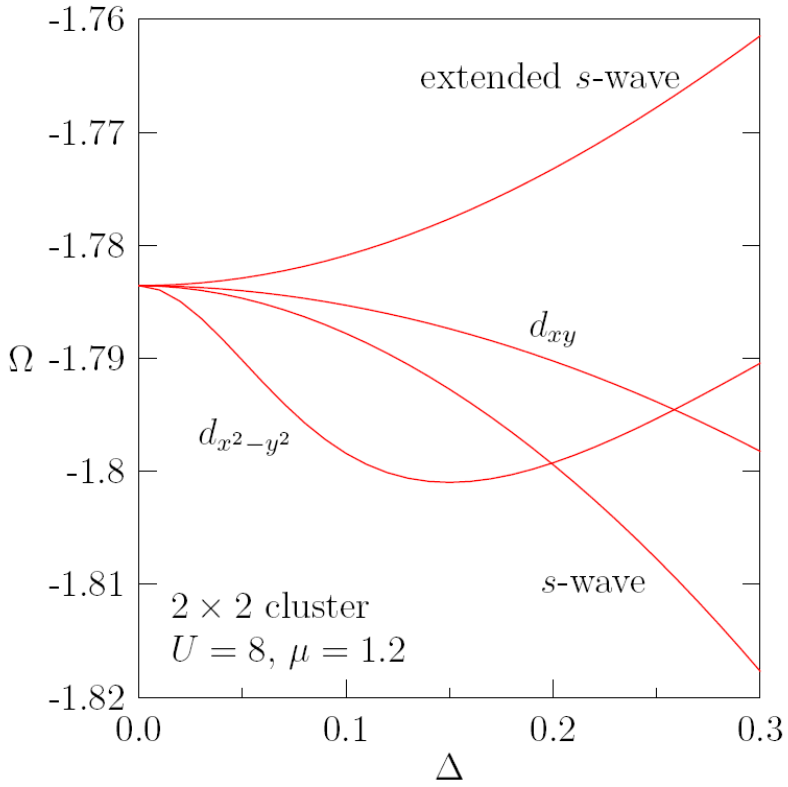
Best scaling factor :

$$q = \frac{\text{number of links}}{2 \times \text{number of sites}}$$

VCA : Superconductivity

The Weiss field is a pairing field

$$\mathcal{O}_{\rm sc} = \sum_{ij} \Delta_{ij} c_{i\uparrow} c_{j\downarrow} + \text{H.c}$$



- *s*-wave

$$\Delta_{ij} = \delta_{ij}$$

- *d*-wave

$$d_{x^2\text{-}y^2} \quad \Delta_{ij} = \begin{cases} 1 & \text{if} \quad \mathbf{r}_i - \mathbf{r}_j = \pm\hat{\mathbf{x}} \\ -1 & \text{if} \quad \mathbf{r}_i - \mathbf{r}_j = \pm\hat{\mathbf{y}} \end{cases}$$

$$d_{xy} \qquad \Delta_{ij} = \begin{cases} 1 & \text{if} \quad \mathbf{r}_i - \mathbf{r}_j = \pm(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \\ -1 & \text{if} \quad \mathbf{r}_i - \mathbf{r}_j = \pm(\hat{\mathbf{x}} - \hat{\mathbf{y}}) \end{cases}$$

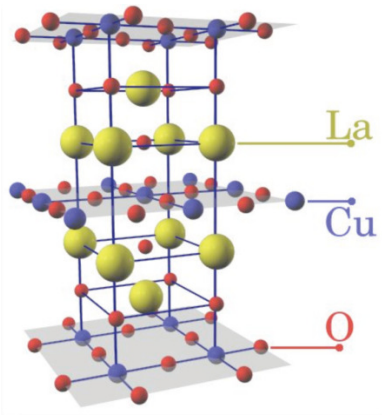
VCA : Superconductivity

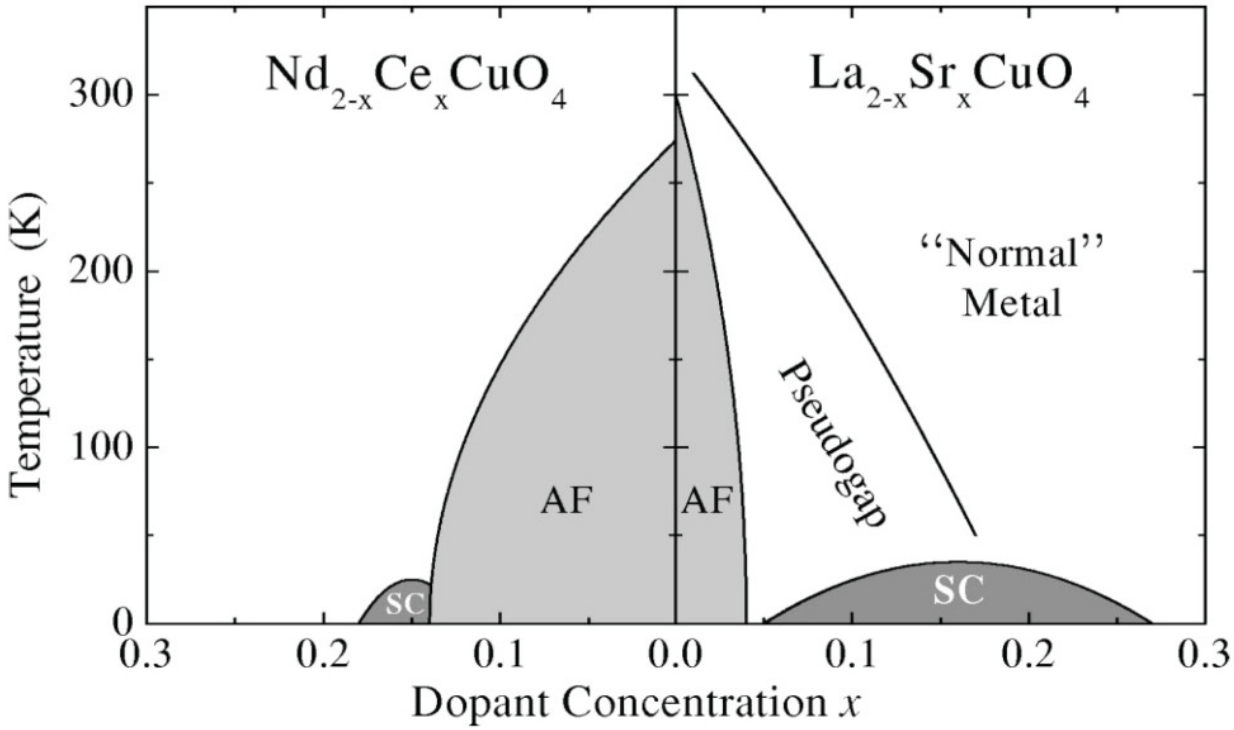
- particle number is not conserved now
- The Hilbert space is enlarged
- *Nambu* formalism is used

$$c_a = c_{a\uparrow} \qquad\qquad d_a = c^{\dagger}_{a\downarrow}$$

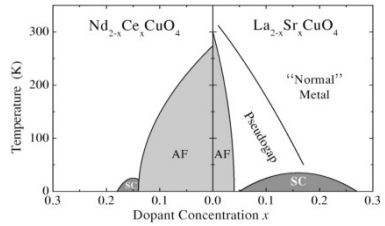
Structure and Phase Diagram

- High T_c superconductors

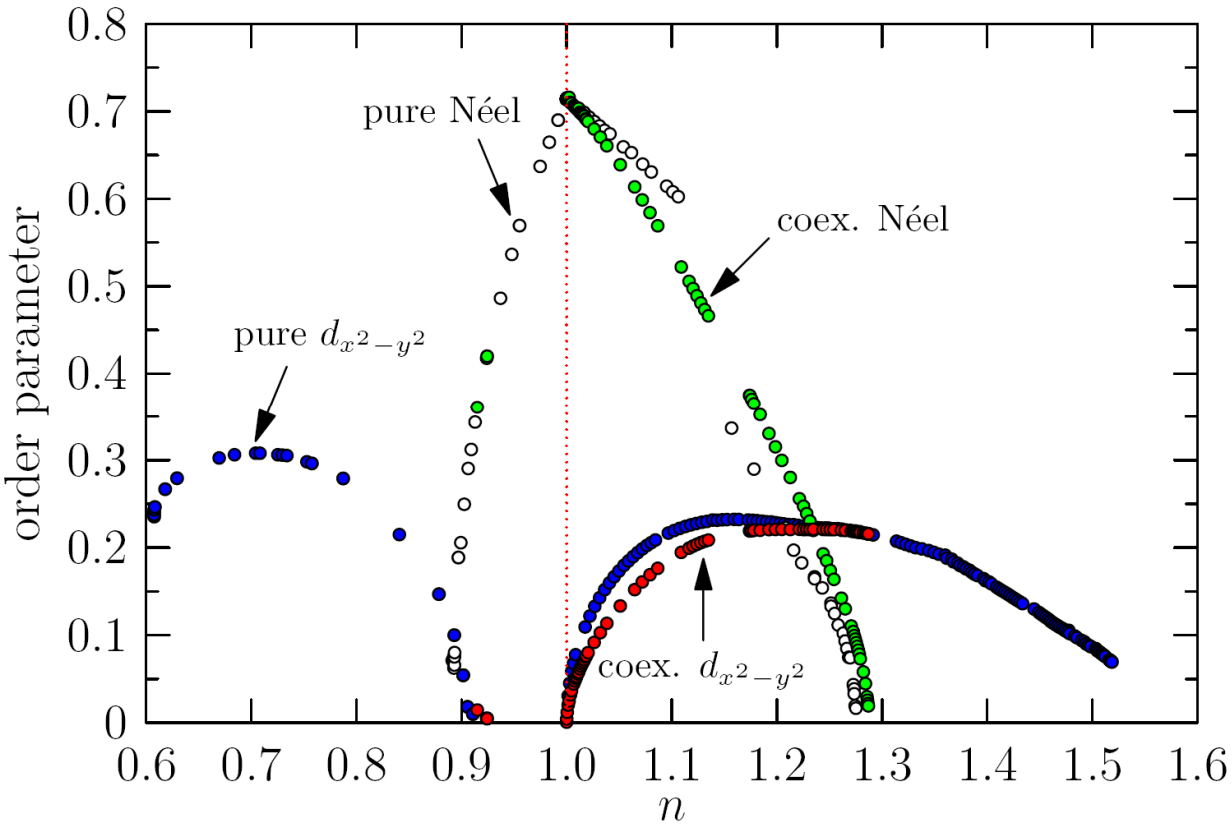




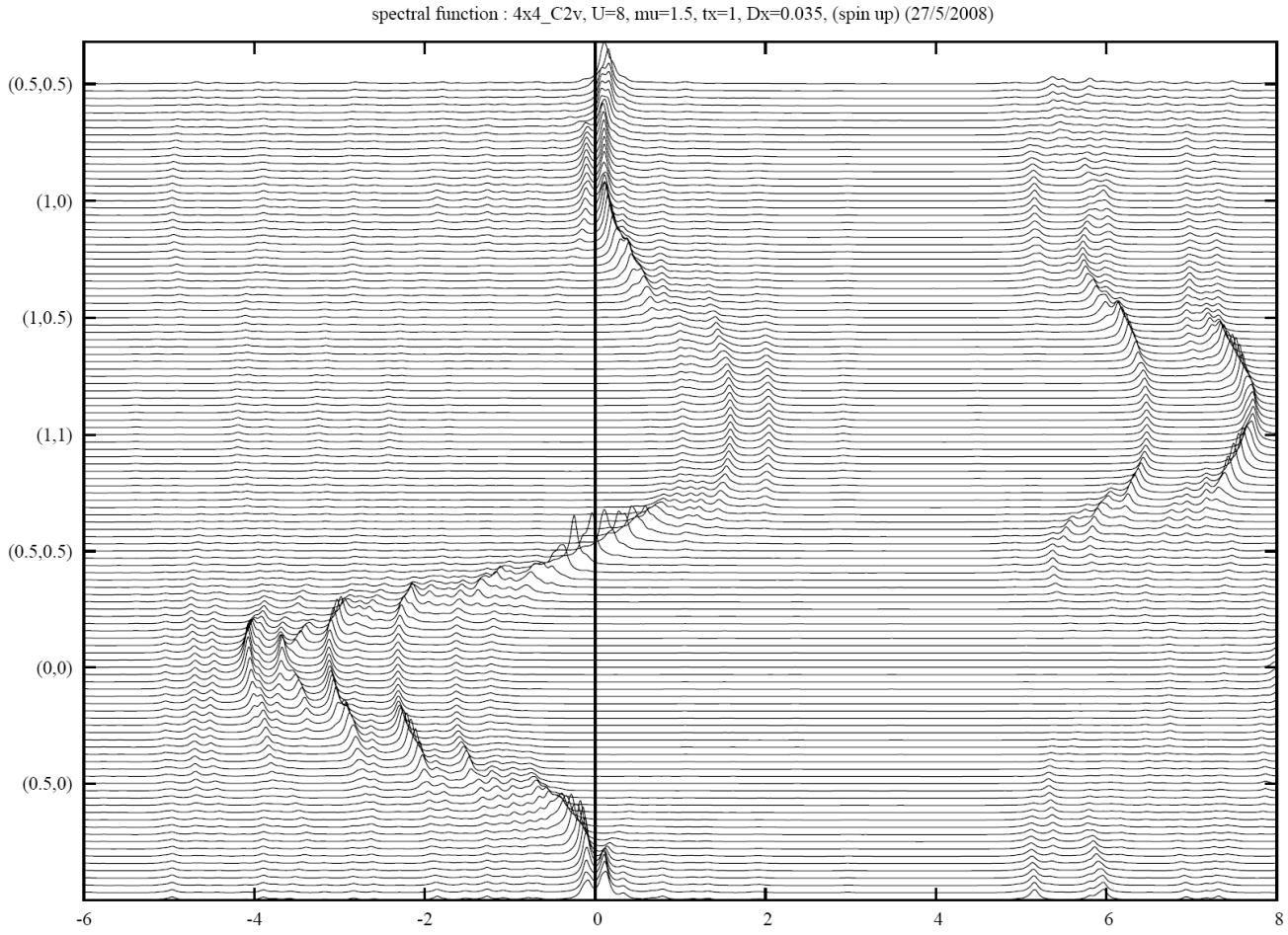
VCA : High T_c superconductors



One-band Hubbard model for the cuprates: t' = -0.3, t'' = 0.2, U = 8:

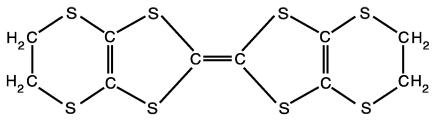


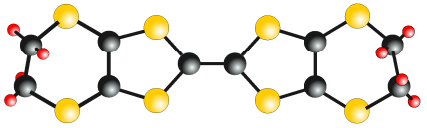
VCA : High T_c superconductors



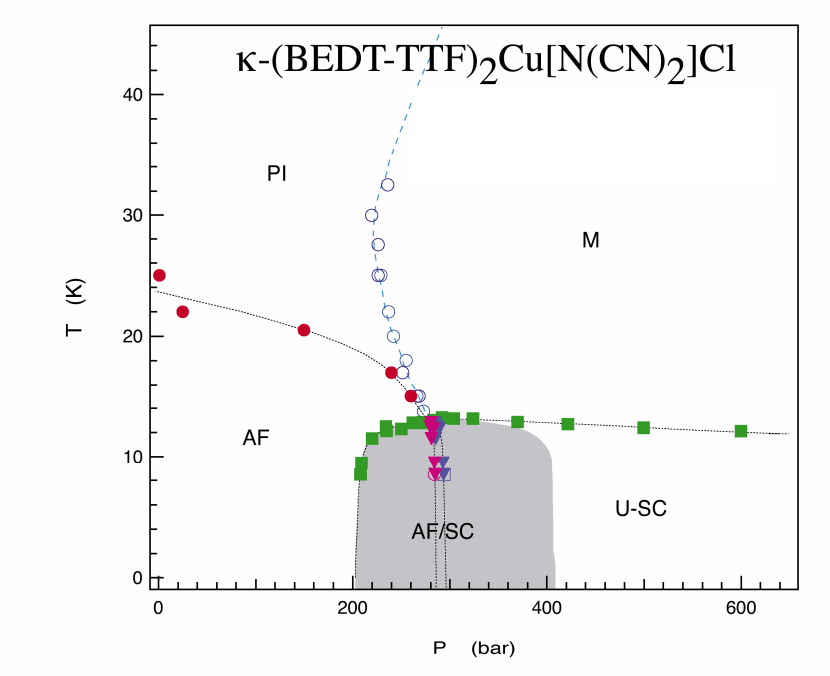
Structure and Phase Diagram

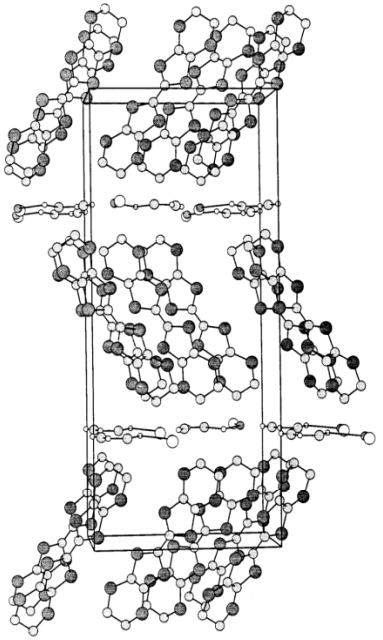
- Organic compounds



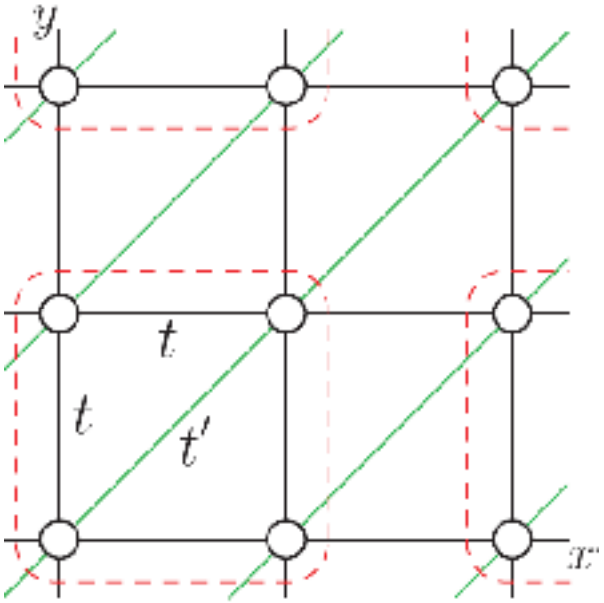


BEDT-TTF (ET)





Structure and Phase Diagram

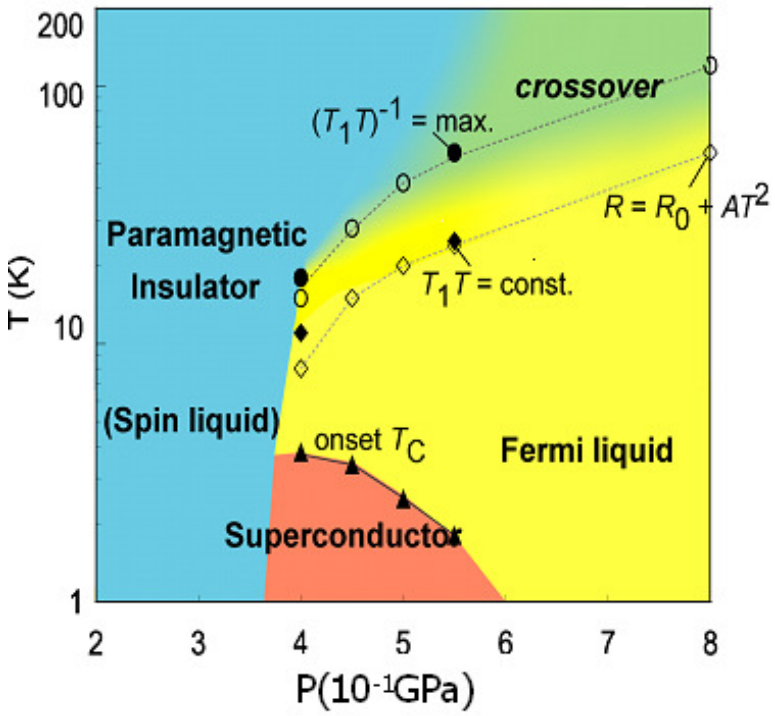


κ-$(ET)_2X$

X^-	Ground State	t'/t
$Cu_2(CN)_3$	Mott insulator	1.06
$Cu[N(CN)_2]Cl$	Mott insulator	0.75
$Cu[N(CN)_2]Br$	SC	0.68
$Cu(NCS)_2$	SC	0.84
$Cu(CN)[N(CN)_2]$	SC	0.68
$Ag(CN)_2 H_2O$	SC	0.60
I_3	SC	0.58

Structure and Phase Diagram

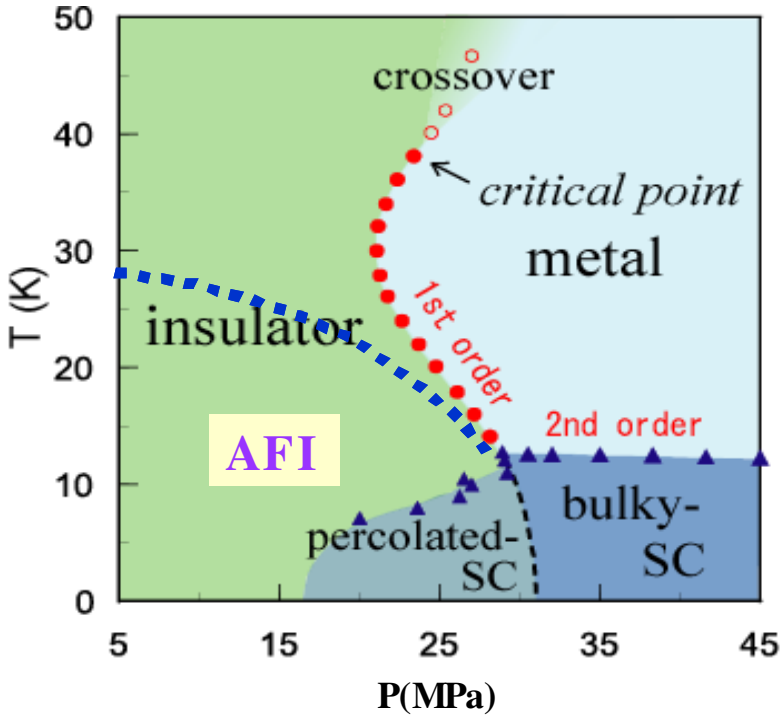
Q2D - SL
κ- $Cu_2(CN)_3$



SL ⟷ d-SC

Kurosaki, PRL95, 2005

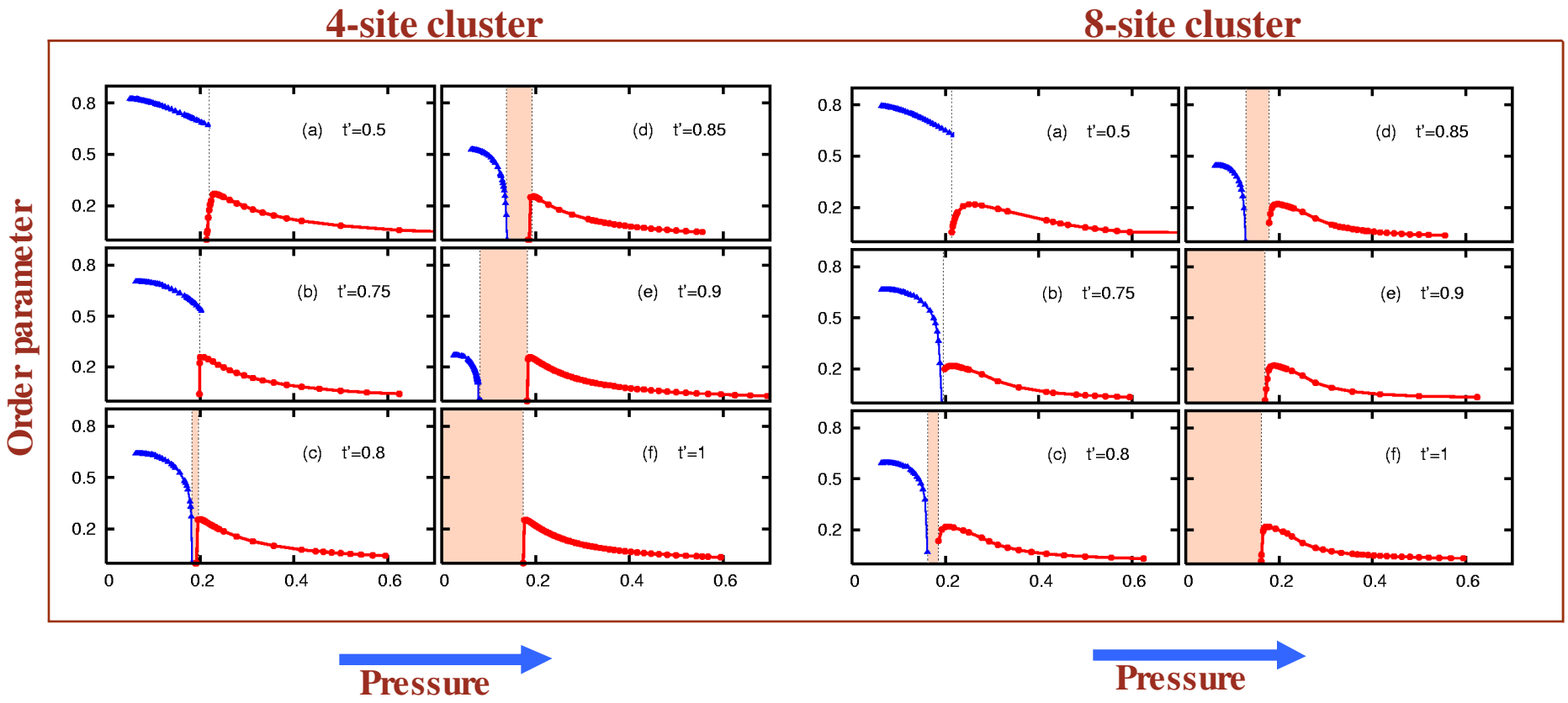
Q2D – AF
κ- $Cu[N(CN)_2]Cl$



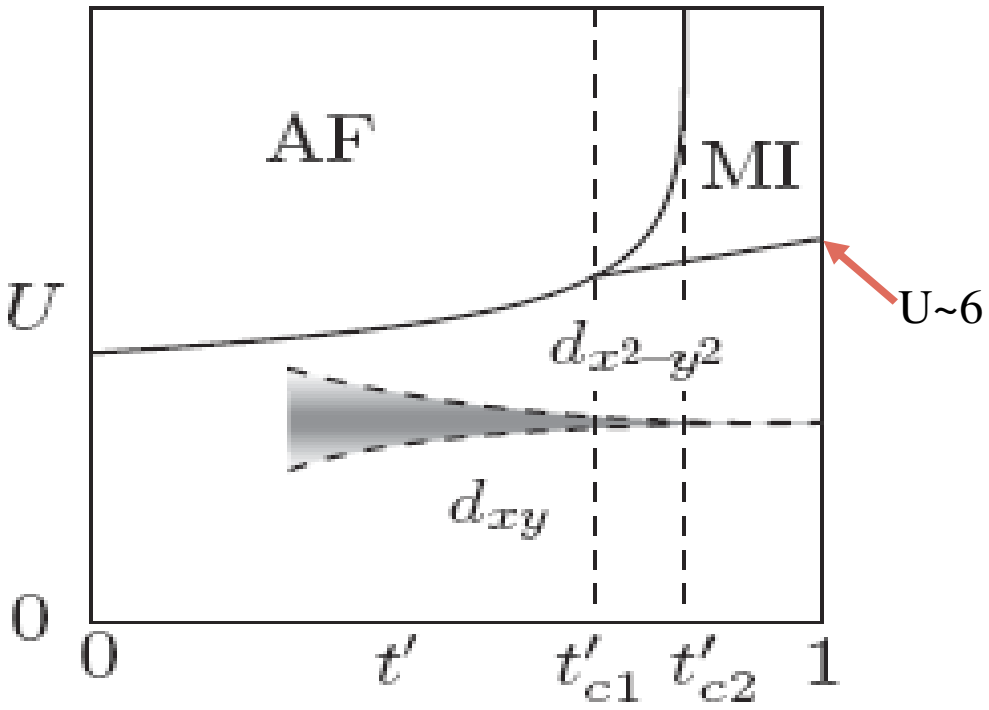
AF ⟷ d-SC

Kagawa, PRB69, 2004

VCA : Organic compounds

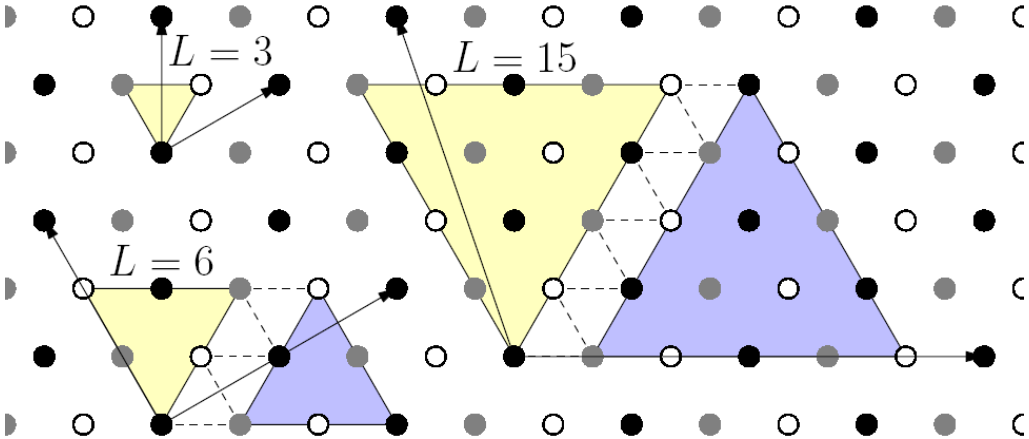


VCA : Organic compounds



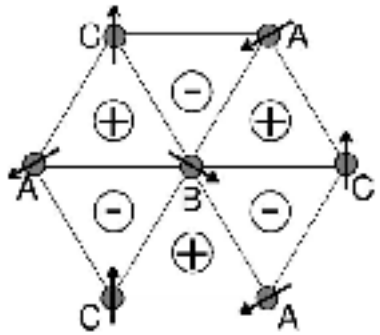
P. Sahebsara, and D. Sénéchal, PRL97 2006

VCA : Organic compounds



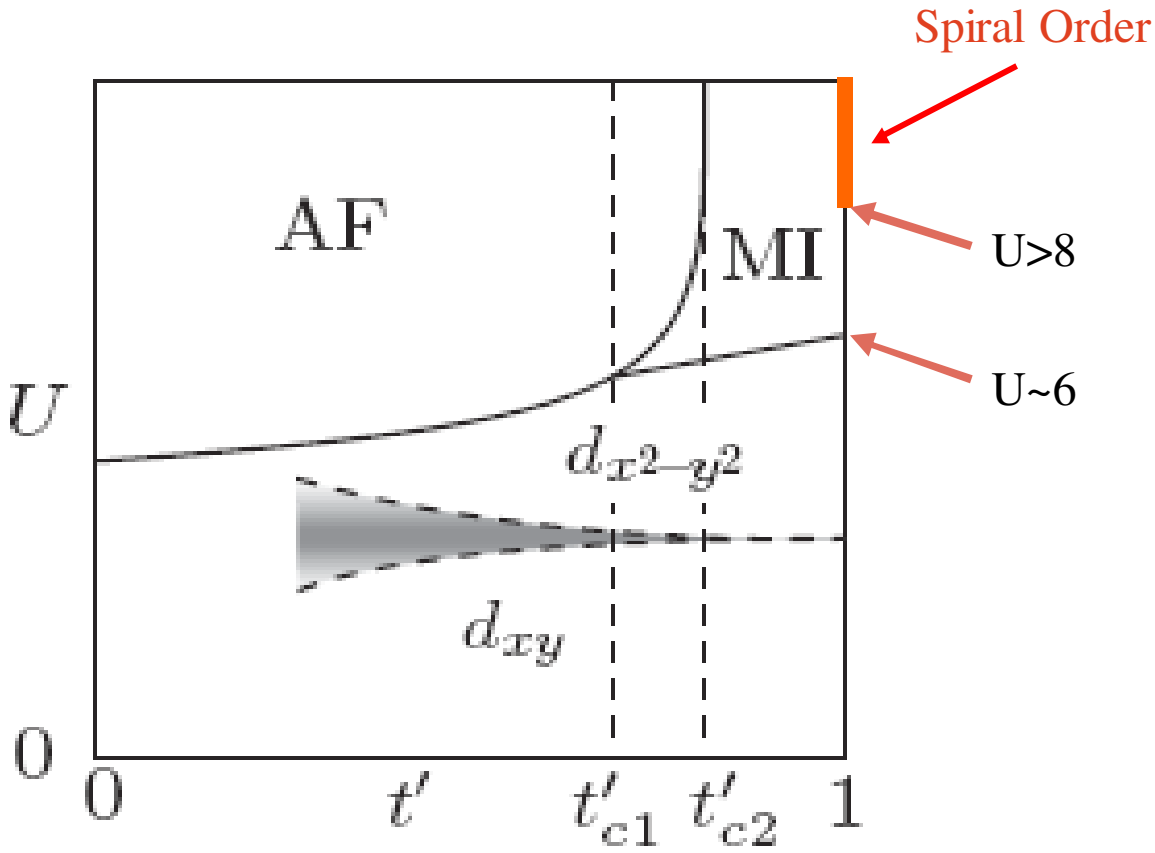
Spiral order

$$H'_{120^\circ} = h\left\{\sum_{i\in A} e_A.S_i + \sum_{i\in B} e_B.S_i + \sum_{i\in C} e_C.S_i\right\}$$

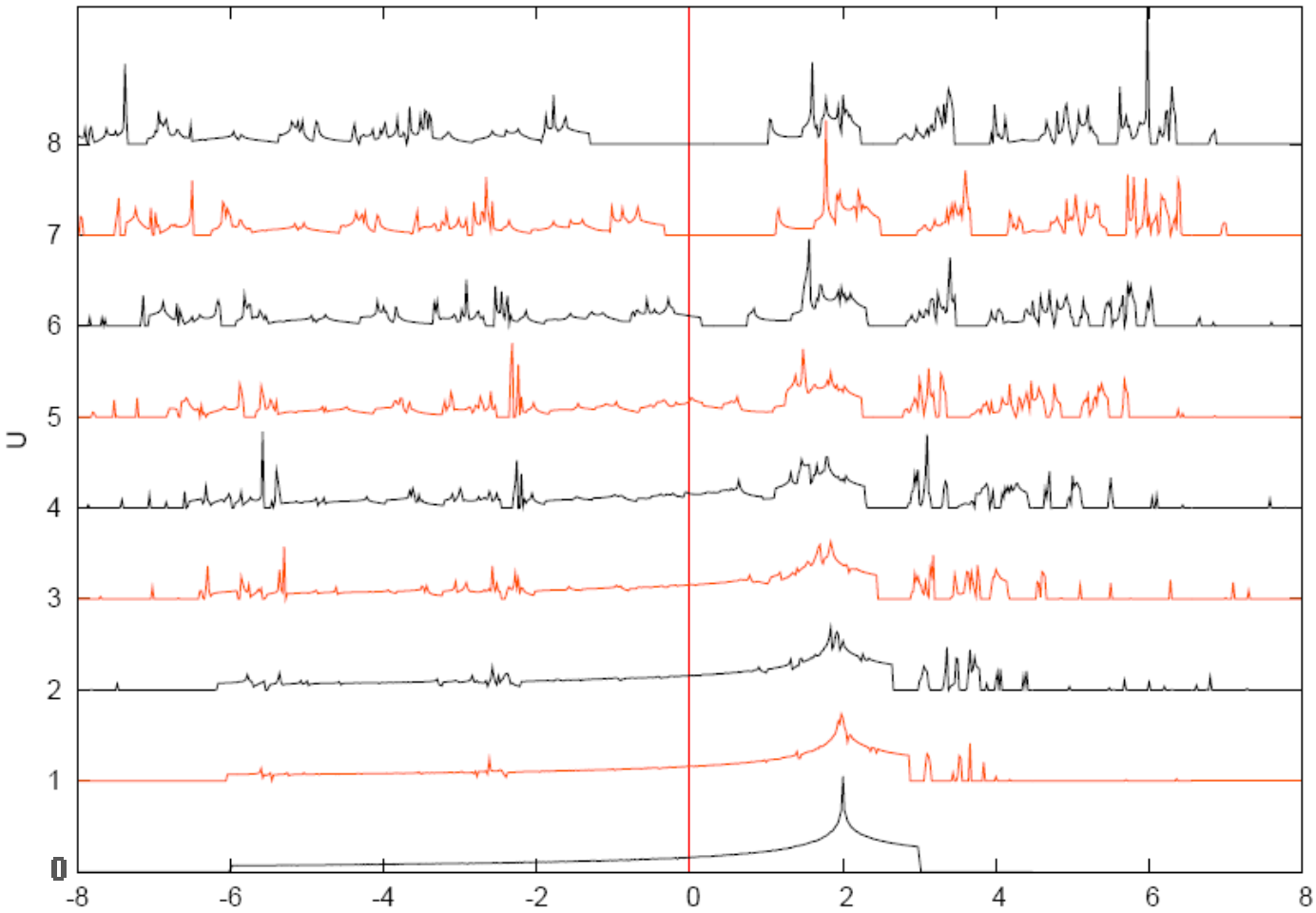


VCA : Organic compounds

VCA

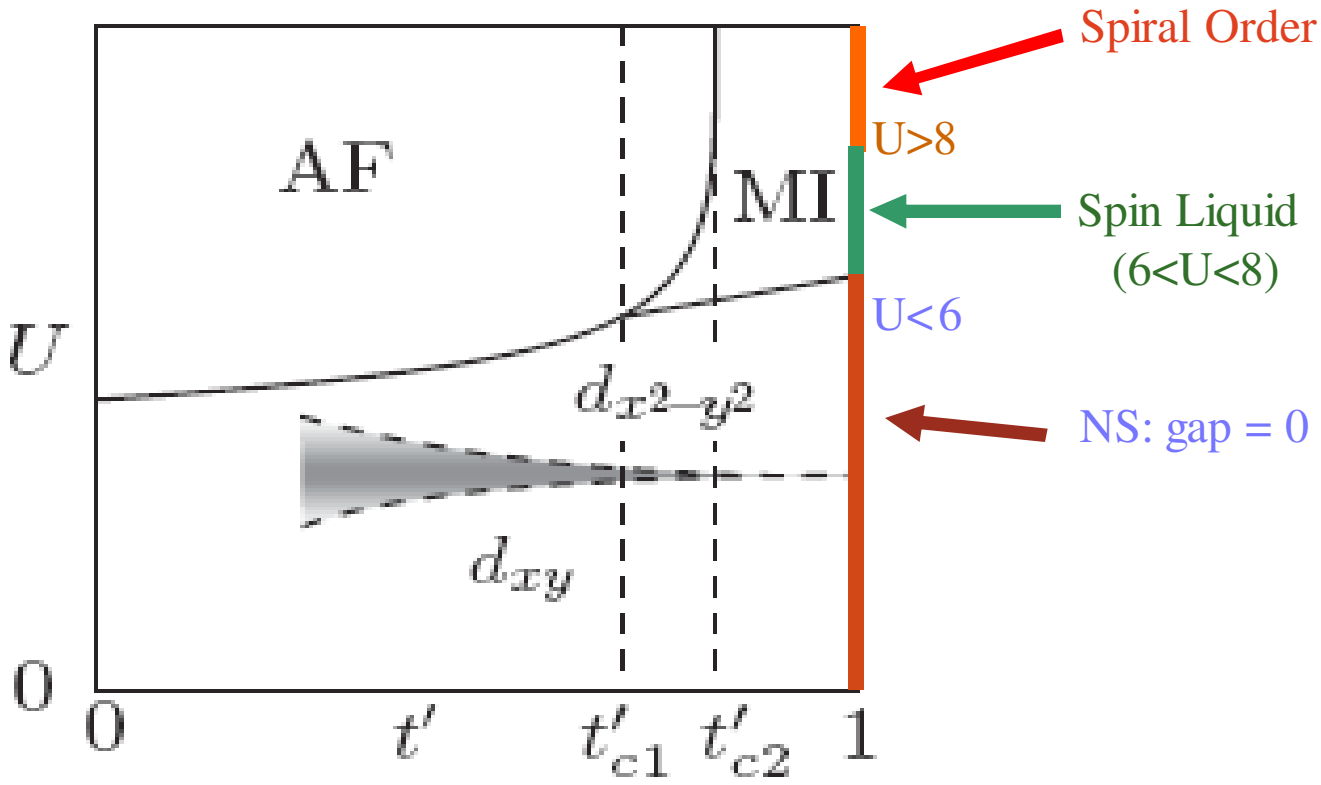


VCA : Organic compounds



P. Sahebsara, IJPR, in press

VCA : Organic compounds



P. Sahebsara, and D. Sénéchal, PRL100, 2008

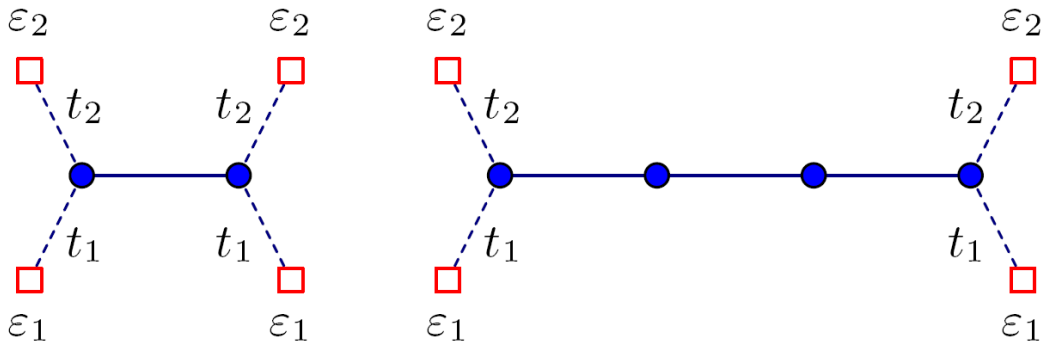
Cluster Dynamical Mean Field Theory

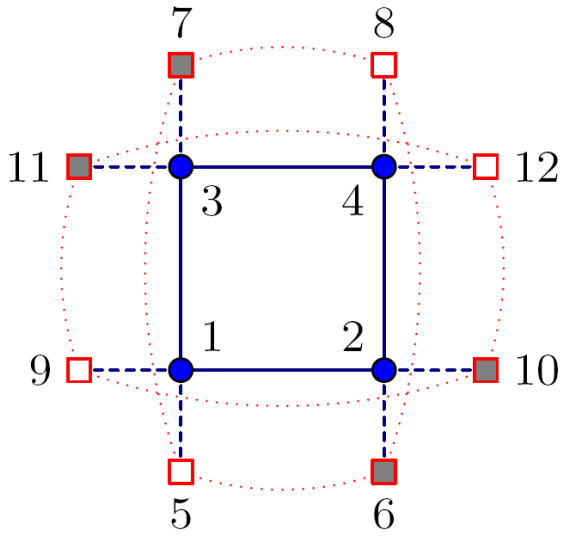
CDMFT : Basic Idea

- To add variational degrees of freedom in the form of a bath of uncorrelated sites

$$H' = -\sum_{\mu,\nu} t_{\mu\nu} c^\dagger_\mu c_\nu + U \sum_a n_{a\uparrow} n_{a\downarrow}$$
$$+ \sum_{\mu,\alpha} \theta_{\mu\alpha} (c^\dagger_\mu a_\alpha + \text{H.c.}) + \sum_\alpha \varepsilon_\alpha a^\dagger_\alpha a_a$$

$\theta_{\mu\alpha}$: hybridization matrix; ε_α: bath energies





CDMFT : The hybridization function

- the cluster Green function takes the form

$$\mathsf{G}'^{-1} = \omega - \mathsf{t} - \mathsf{\Gamma}(\omega) - \mathsf{\Sigma}(\omega)$$

- $\Gamma(\omega)$ is the hybridization function:

$$\Gamma_{\mu\nu}(\omega) = \sum_{\alpha} \frac{\theta_{\mu\alpha}\theta^{*}_{\nu\alpha}}{\omega - \varepsilon_{\alpha}}$$

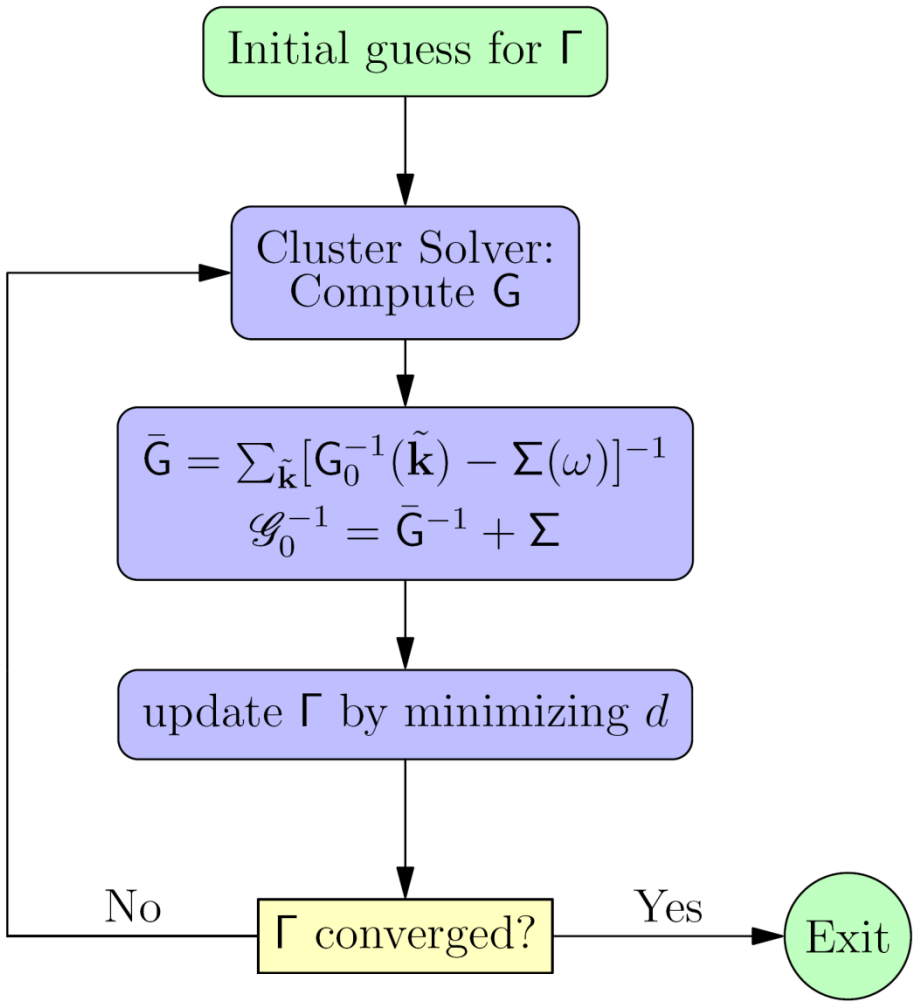
CDMFT : The hybridization function

- The bath makes a contribution to the Potthoff functional:

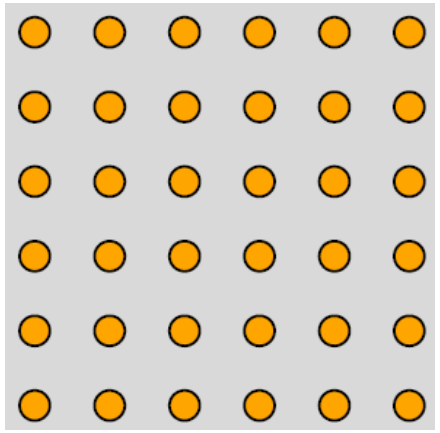
$$\Omega_{\mathrm{bath}} = \sum_{\varepsilon_\alpha < 0} \varepsilon_\alpha$$

- On can in principle use the same methods as in VCA

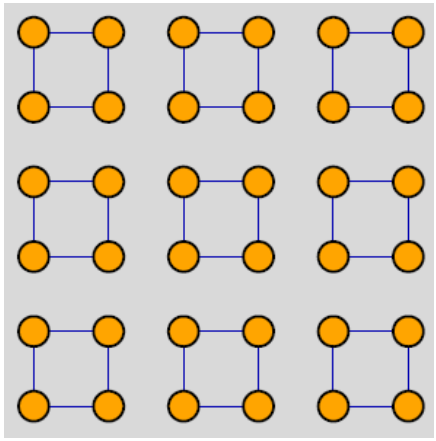
CDMFT : The Algorithm



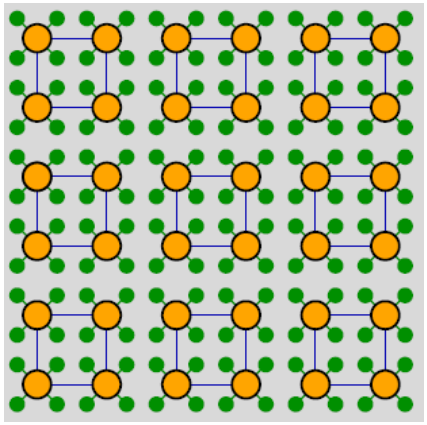
Summary



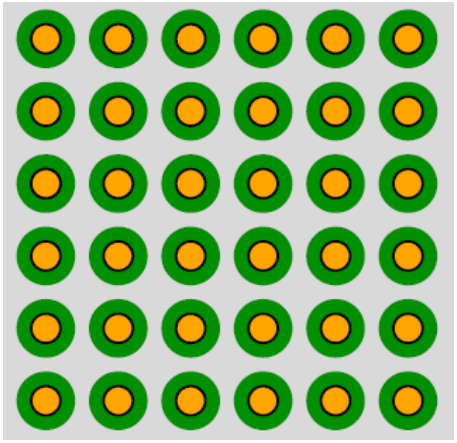
Original system



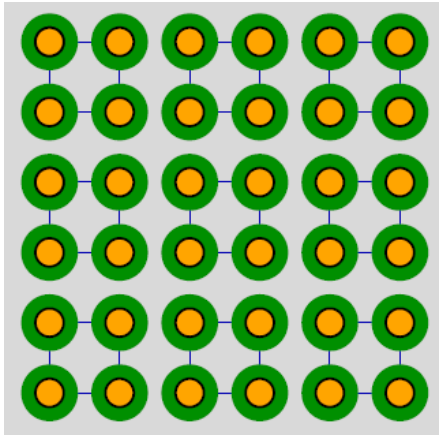
CPT - VCA



VCA + CDMFT



DMFT



C-DMFT

... and life is going on!

Thank you