Strongly-coupled superconductivity from quantum cluster approaches

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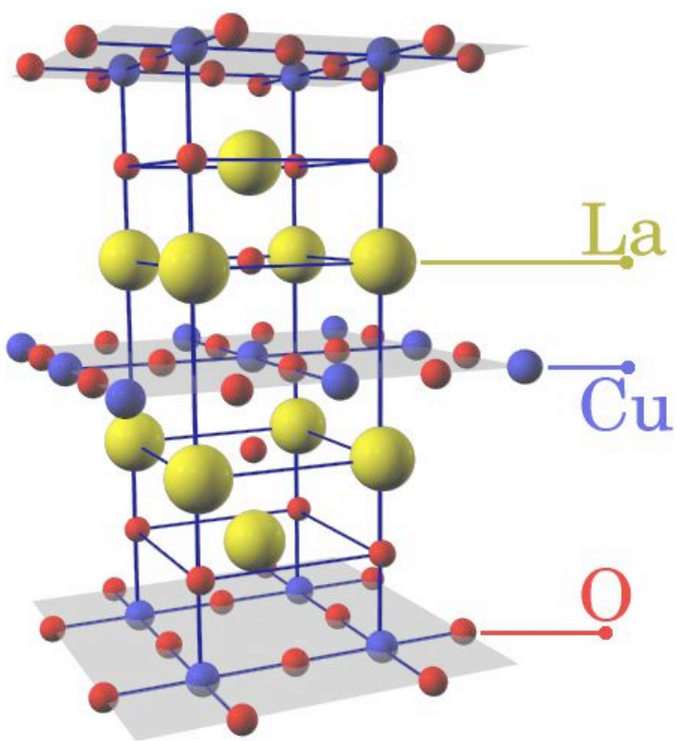
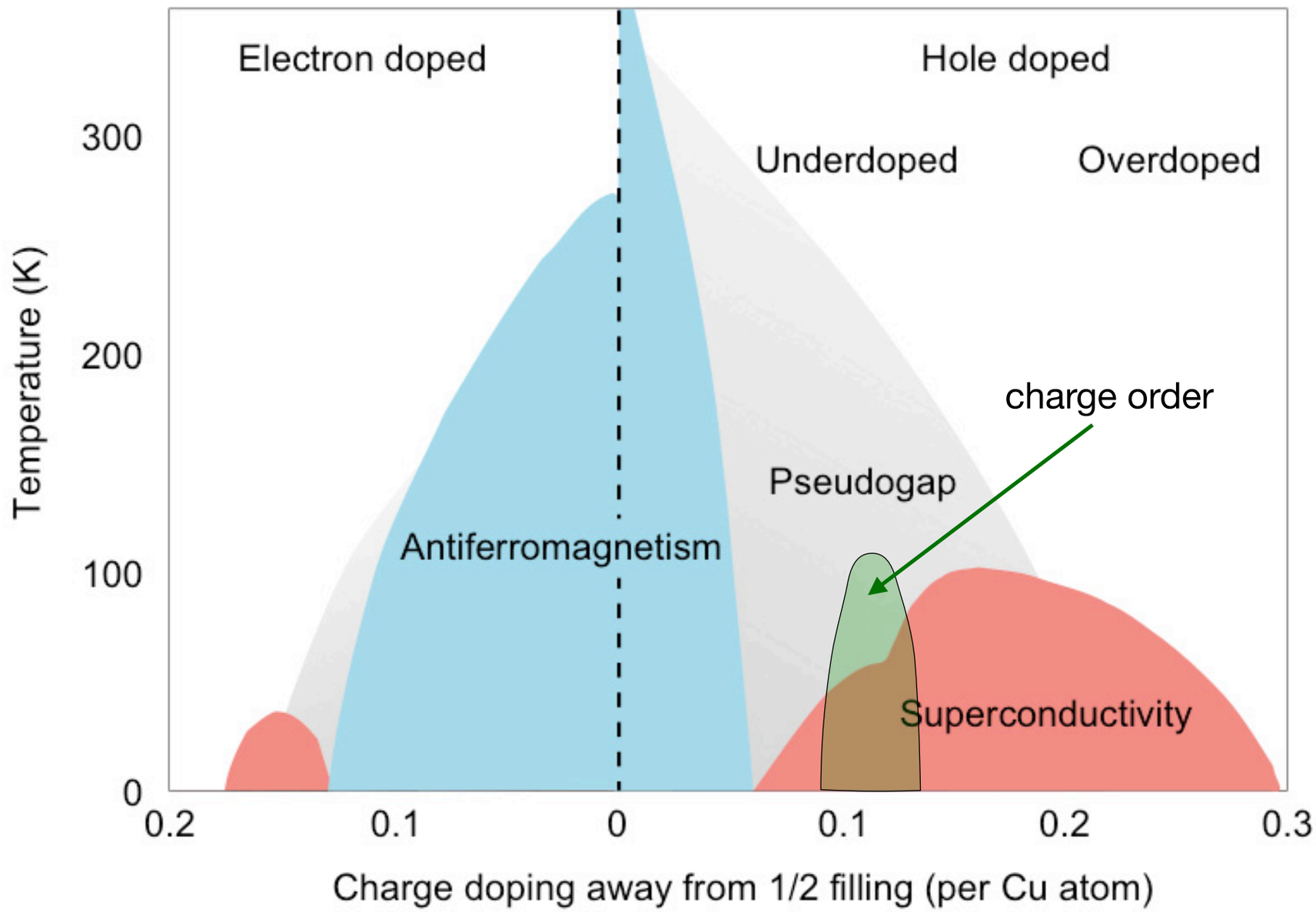
Outline

- Hubbard models
- Quantum cluster methods :
  - VCA (variational cluster approximation)
  - CDMFT (cluster dynamical mean field theory)
- Superconductivity in cuprates from CDMFT
  - 1-band Hubbard model
  - 3-band Hubbard model
- Charge order in cuprates
- Loop currents

High-T_c superconductors





http://www.mrsec.umn.edu/research/seeds/2011/greven2011.html

The Hubbard model

hopping amplitude

number of spin ↑ electrons at $\mathbf{r}$

$$H = \sum_{\mathbf{r},\mathbf{r}',\sigma} t_{\mathbf{r},\mathbf{r}'} c^{\dagger}_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} - \mu \sum_{\mathbf{r},\sigma} n_{\mathbf{r},\sigma}$$

creation operator

repulsion

- Simplest model for strong correlations
- AF phase at half-filling + Mott at higher temperature
- Paradigm: *high-Tc superconductors are doped Mott/AF insulators*

- Progress done with quantum cluster methods:
  - Need short-range fluctuations to understand superconductivity
  - Relation with short-range AF fluctuations made evident numerically

The 3-band Hubbard model

creates a p electron ← creates a d electron

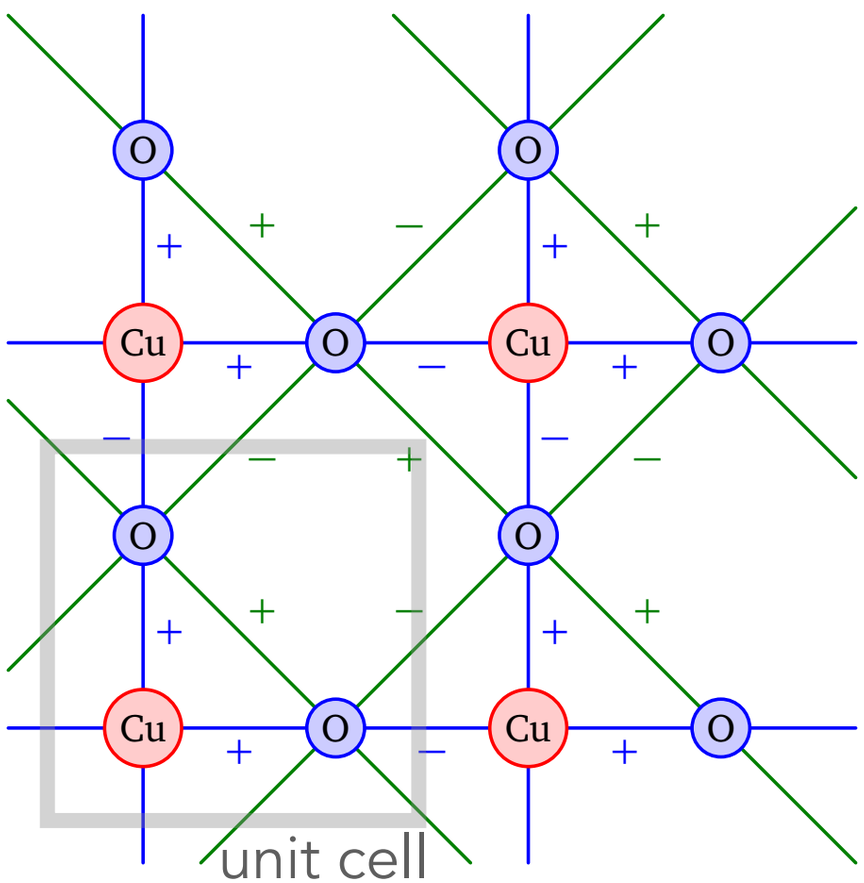
$$H = t_{pd} \sum_{\langle i,j \rangle} \left(p^{\dagger}_{i\sigma} d_{i\sigma} + d^{\dagger}_{i\sigma} p_{j\sigma} \right) + t_{pp} \sum_{\langle j,j' \rangle} \left(p^{\dagger}_{j\sigma} p_{j'\sigma} + \text{H.c.} \right)$$

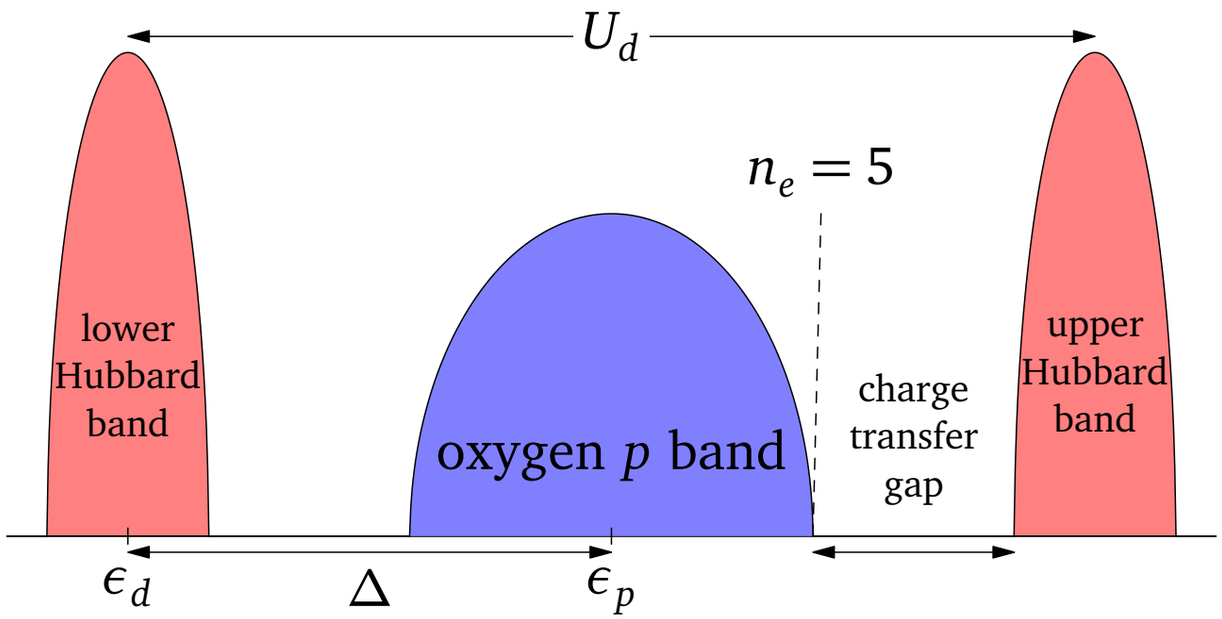
p orbital level

$$+ U_d \sum_{i} n^{(d)}_{i\uparrow} n^{(d)}_{i\downarrow} + (\varepsilon_d - \mu) \sum_{i,\sigma} n^{(d)}_{i\sigma} + (\varepsilon_p - \mu) \sum_{j,\sigma} n^{(p)}_{j\sigma}$$

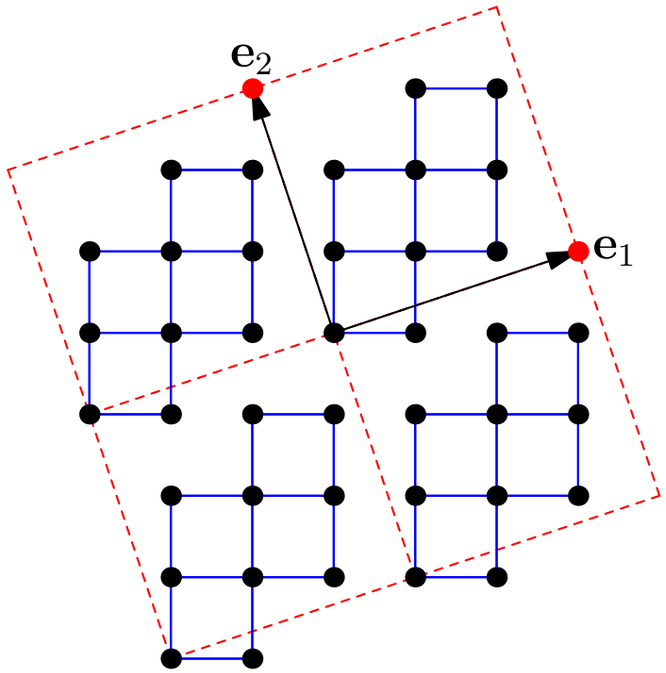
Cu-Cu repulsion

d orbital level

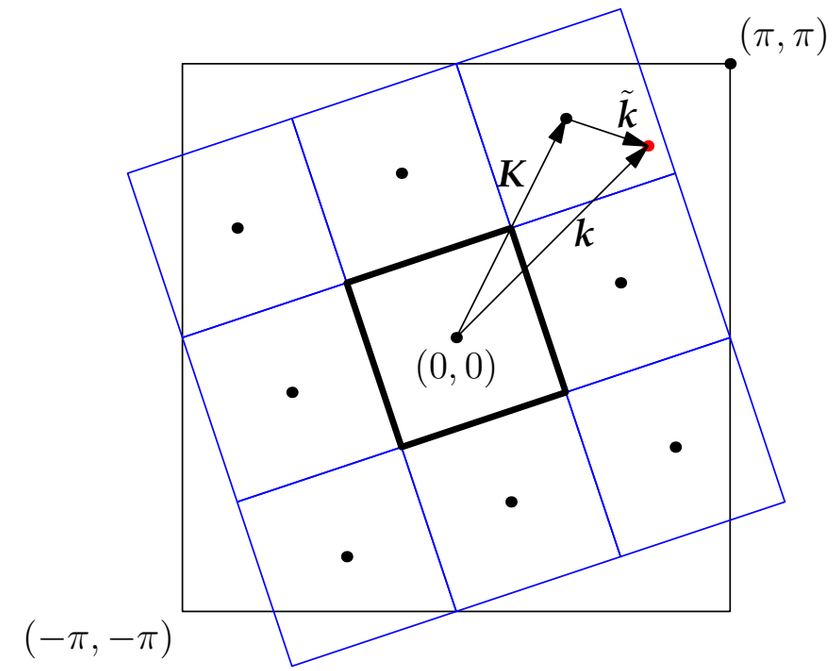




Quantum cluster methods



10-site cluster



Brillouin zones

dispersion relation ← → cluster self-energy

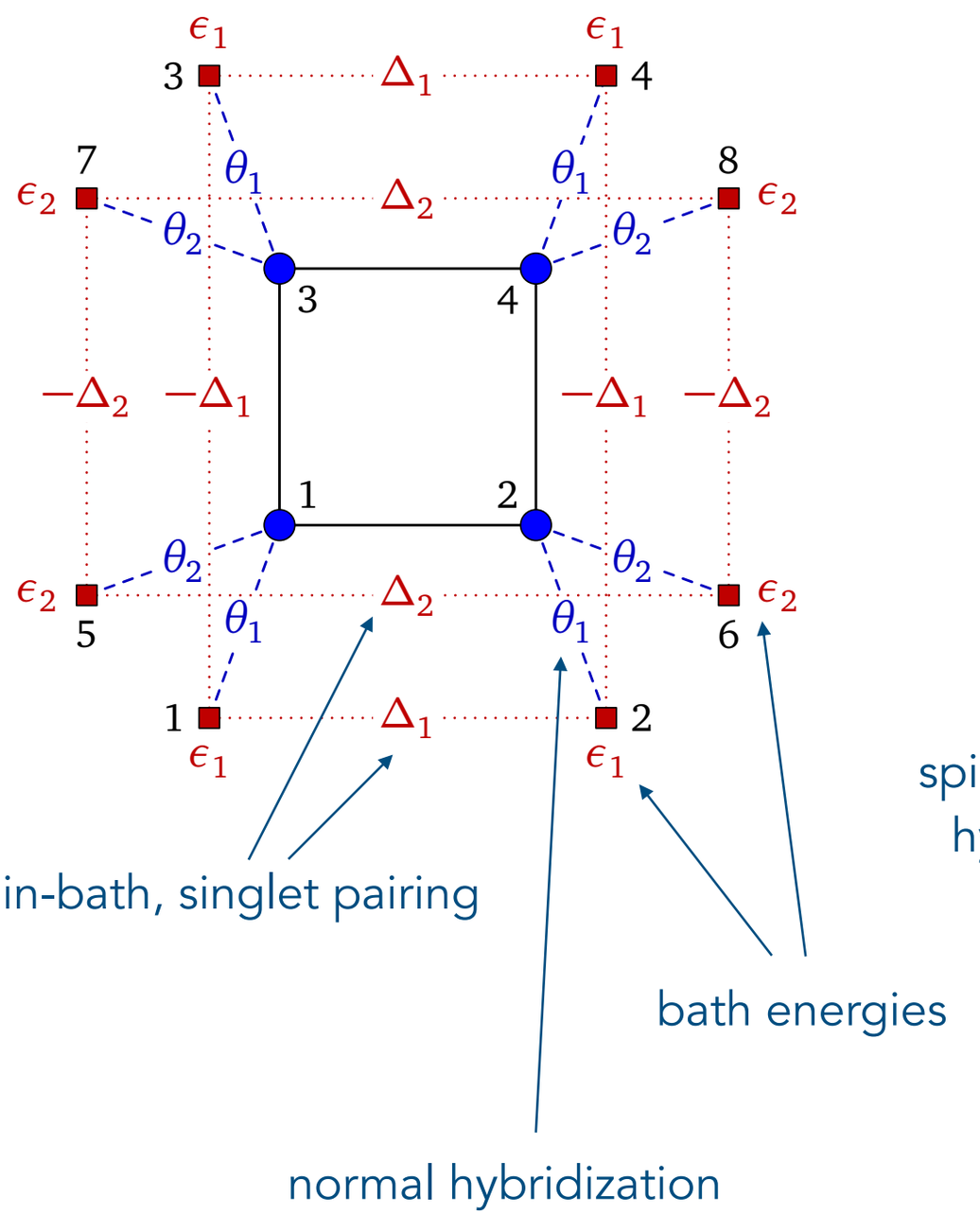
$$\mathbf{G}^{-1}(\tilde{\mathbf{k}}, \omega) = \mathbf{t}(\tilde{\mathbf{k}}) - \boldsymbol{\Sigma}'(\omega)$$

- Based on Green functions
- Lattice tiled by identical units (clusters)
- Clusters used to compute the electron self-energy $\boldsymbol{\Sigma}$, otherwise full lattice dispersion relation used
- Different schemes to embed clusters in the lattice model (VCA, CDMFT,…)
- Different **impurity solvers** (ED, CT-HYB, CT-INT, CT-AUX, …)

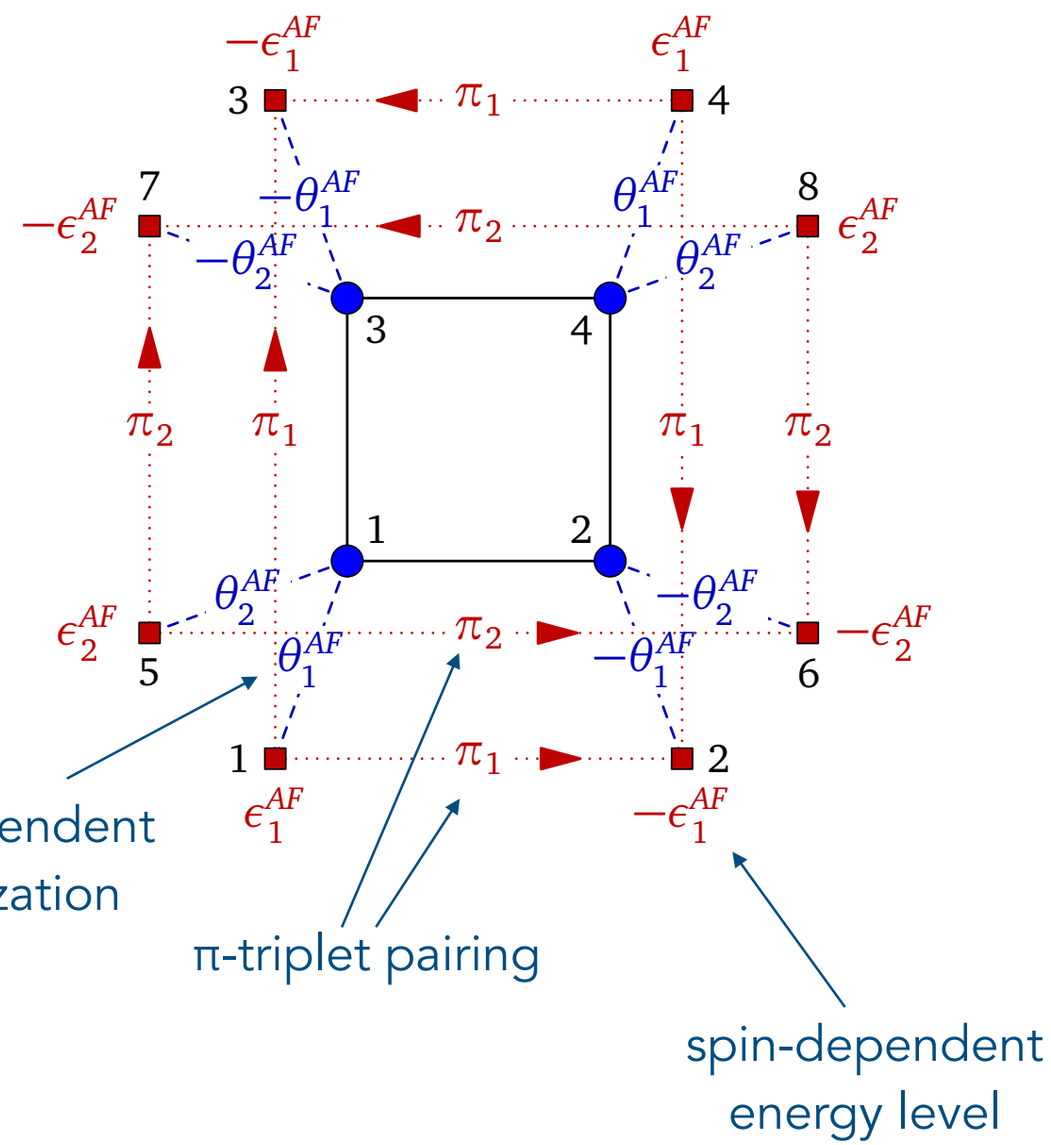
Exact diagonalization at T=0 in this presentation

CDMFT : simple bath parametrization for d-wave SC

pure d-wave SC



d-wave SC + AF

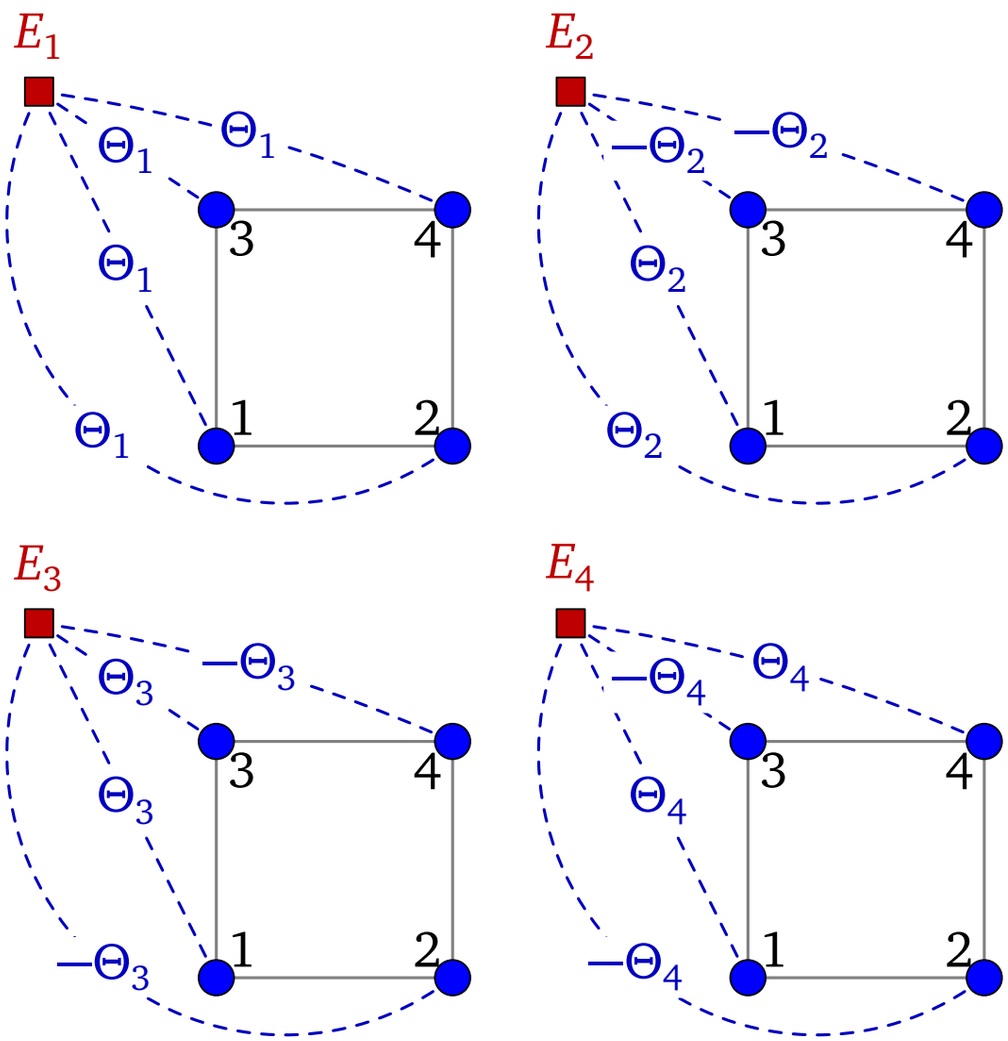


bath is *not* diagonal
6 or 12 parameters

Bath parametrization according to cluster symmetry

pure d-wave SC

C_{2v} : 4 irreducible representations

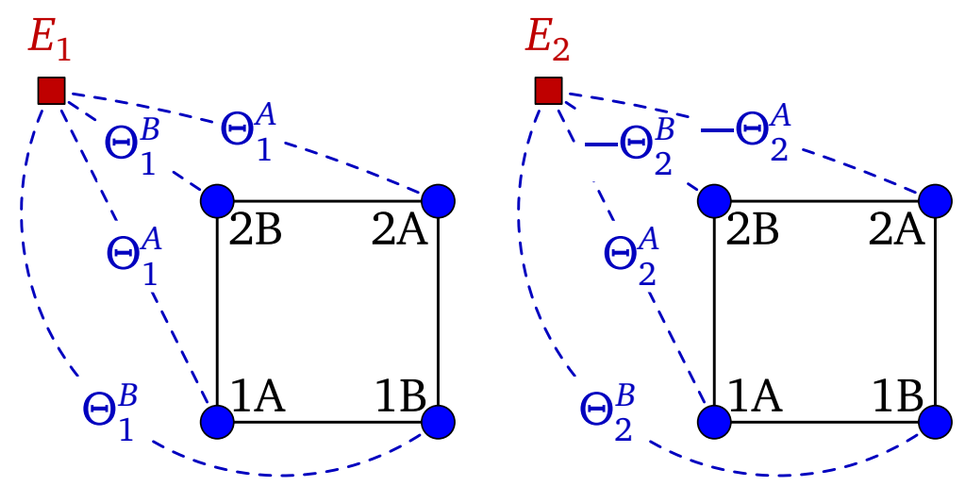


$$E_i \overset{\pm\Theta_i}{\text{- - -}} j \equiv \pm(\theta_i a_i^\dagger c_j + \Delta_i a_i (\mathrm{i}\sigma_y) c_j + \mathrm{H.c.})$$

normal singlet

d-wave SC + AF

C_2 : 2 irreducible representations



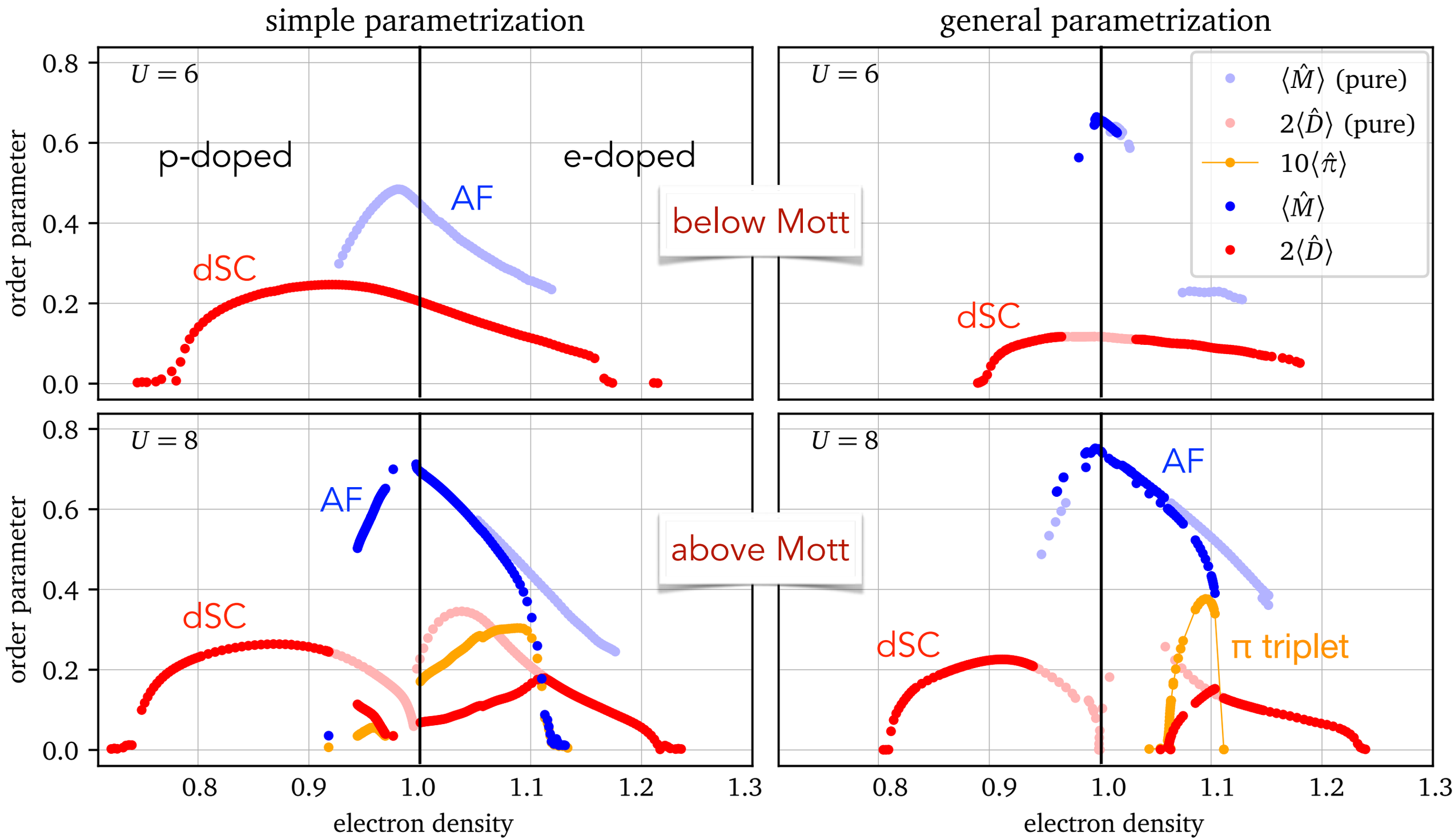
singlet

$$E_i \overset{\pm\Theta_i^X}{\text{- - -}} jX \equiv \pm(\theta_{iX} a_i^\dagger c_{jX} + \Delta_{iX} a_i (\mathrm{i}\sigma_y) c_{jX} + \theta_{iX}^s a_i^\dagger \sigma_z c_{jX} + T_{iX} a_i \sigma_x c_{jX} + \mathrm{H.c.})$$

spin dependent triplet

bath is diagonal
24 or 72 parameters

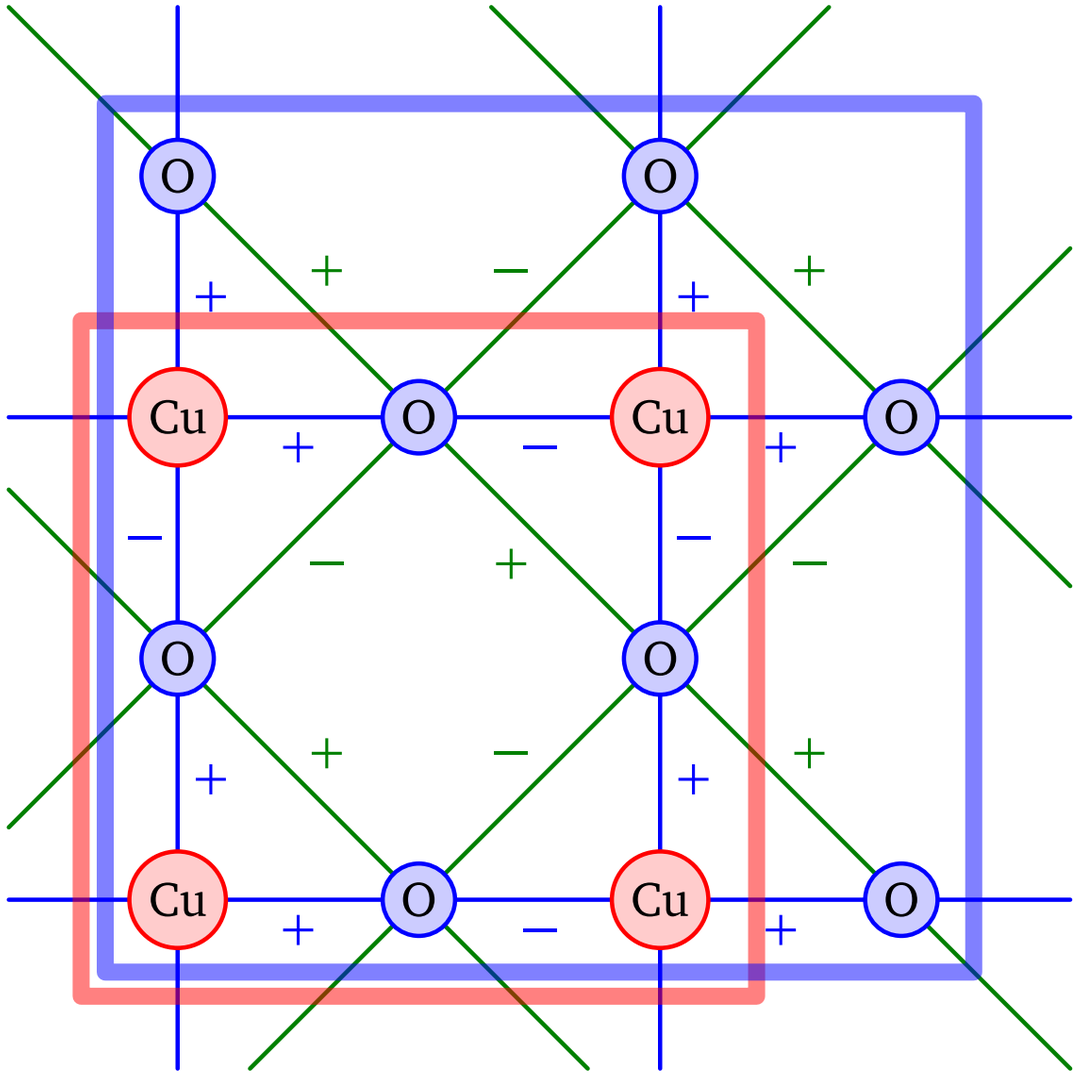
CDMFT : One-band model for YBCO



A. Foley, S. Verret, AM Tremblay & DS, Phys. Rev. B **99**, 184510 (2019)

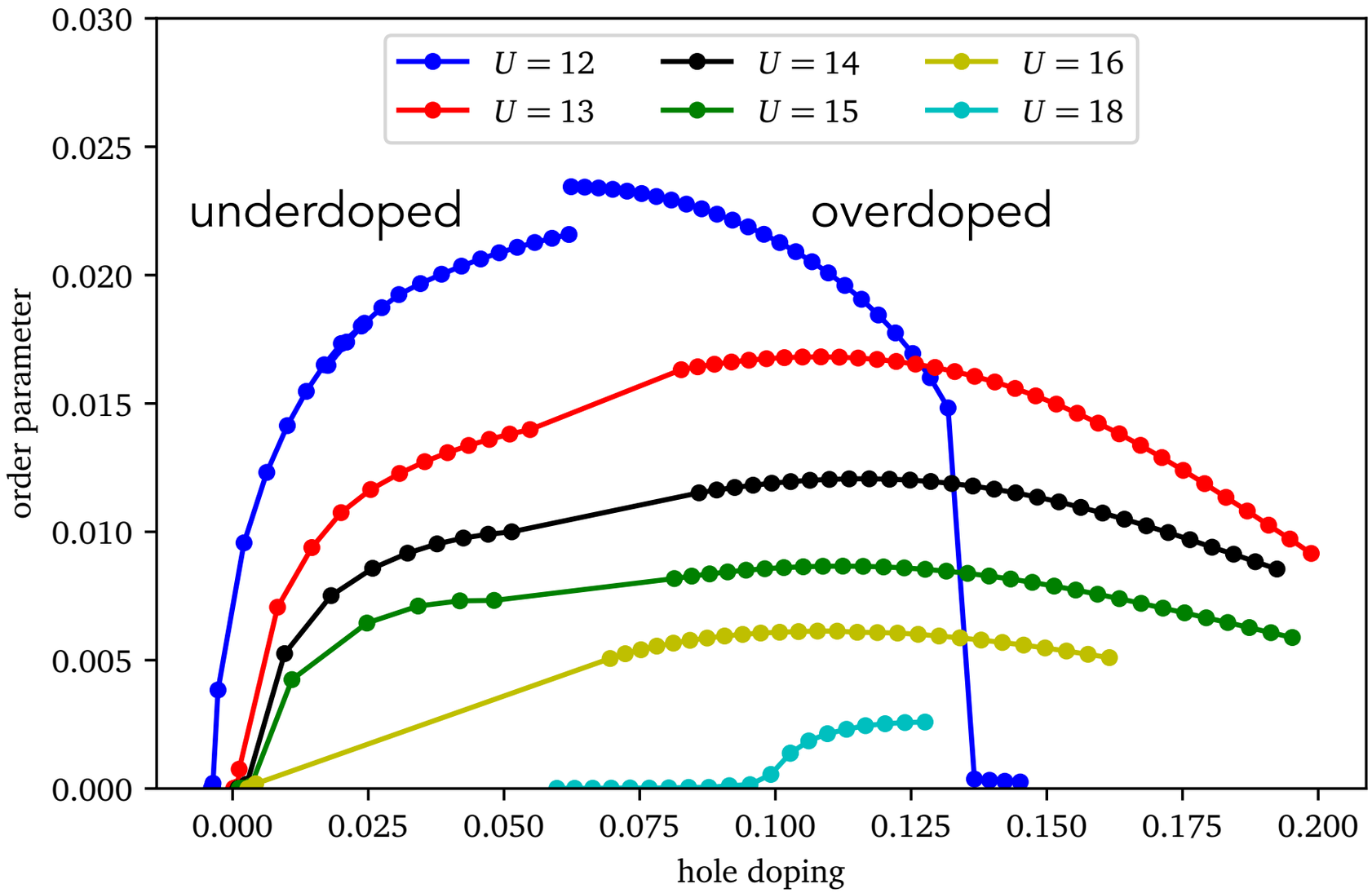
CDMFT and the 3-band model

- Different, overlapping clusters for Cu and O atoms
- General bath parametrization for Cu cluster
- O cluster is non-interacting: acts like a constant hybridization and has effect only via CDMFT self-consistency relation



parameter set: $t_{pp} = 1 \quad t_{pd} = 1.5 \quad \varepsilon_p = 7.0 \quad \varepsilon_d = 0$

3-band model : dSC order parameter (CDMFT)



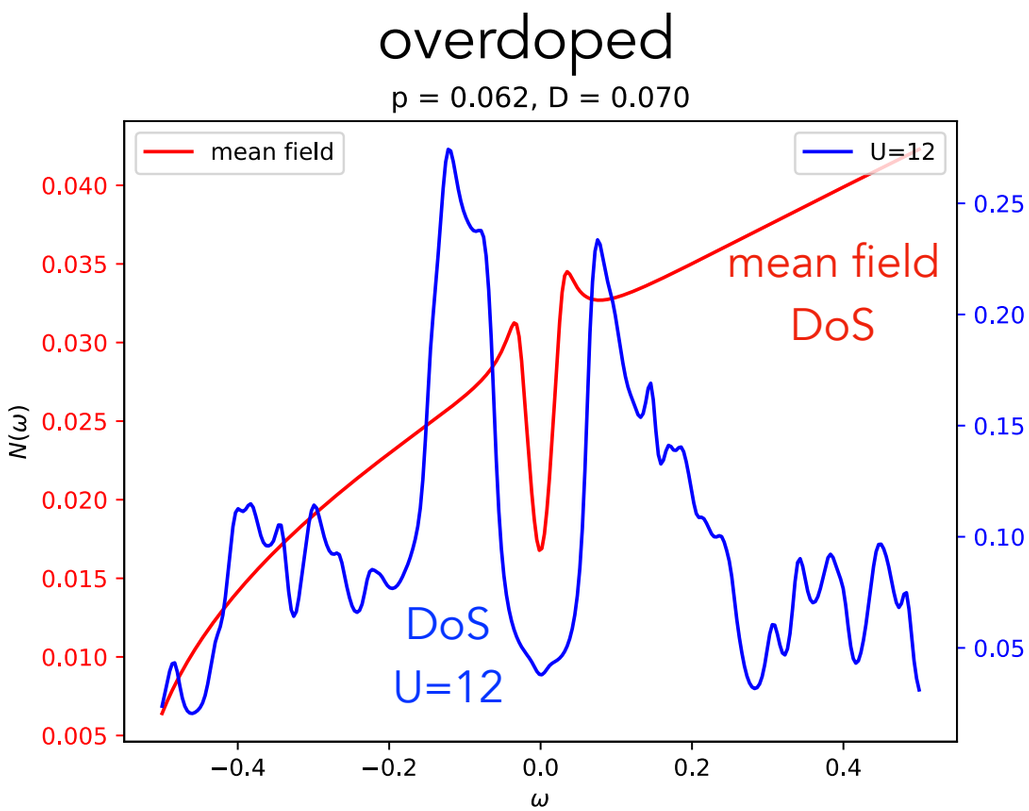
First-order transition between **underdoped** and **overdoped** SC

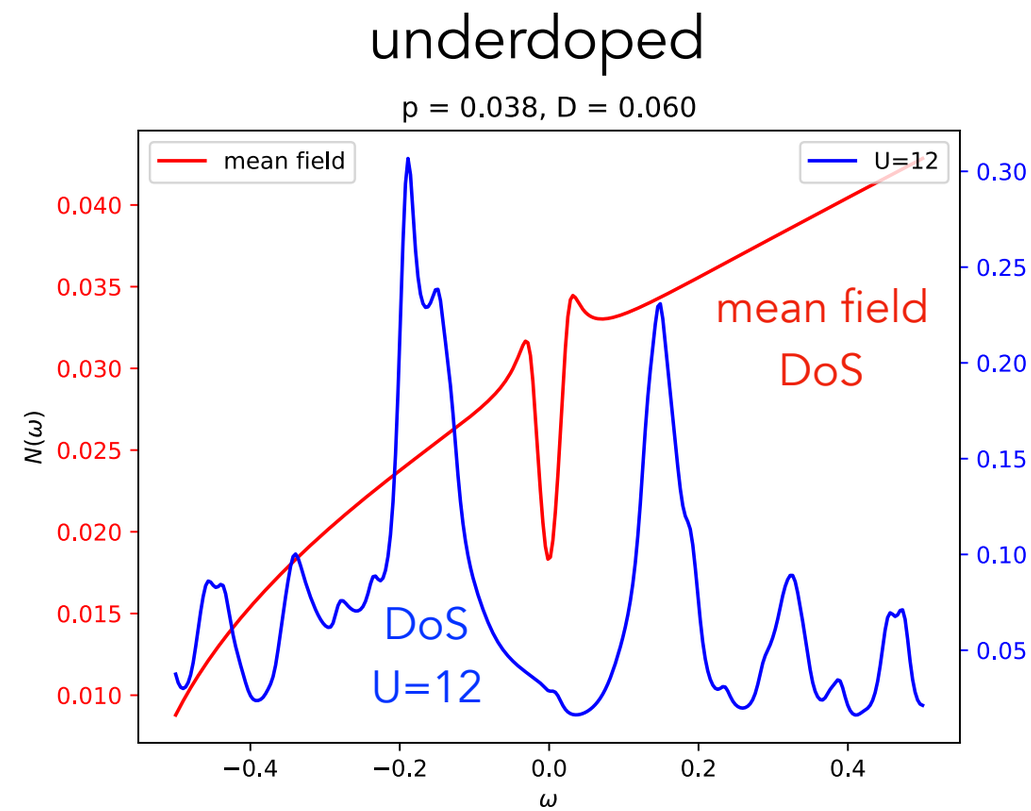
region of coexistence between two SC solutions (**BEC — BCS**)

antiferromagnetism **not** probed in this study

S. Dash & DS, in preparation

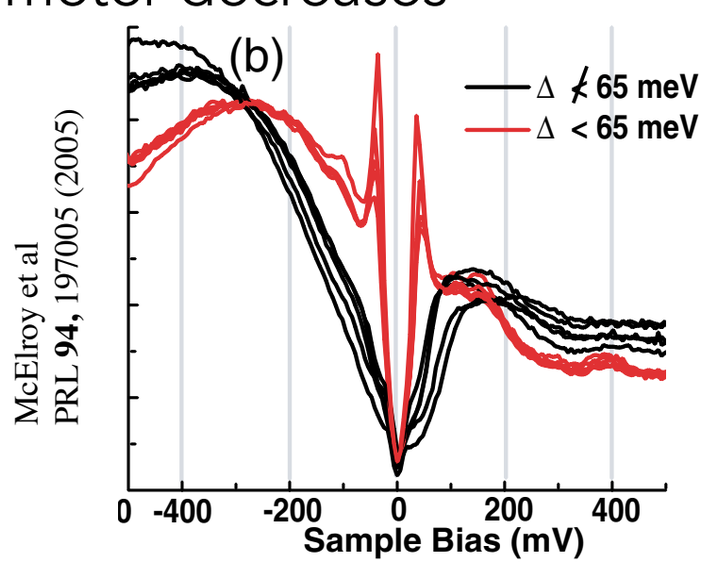
3-band model : underdoped vs overdoped

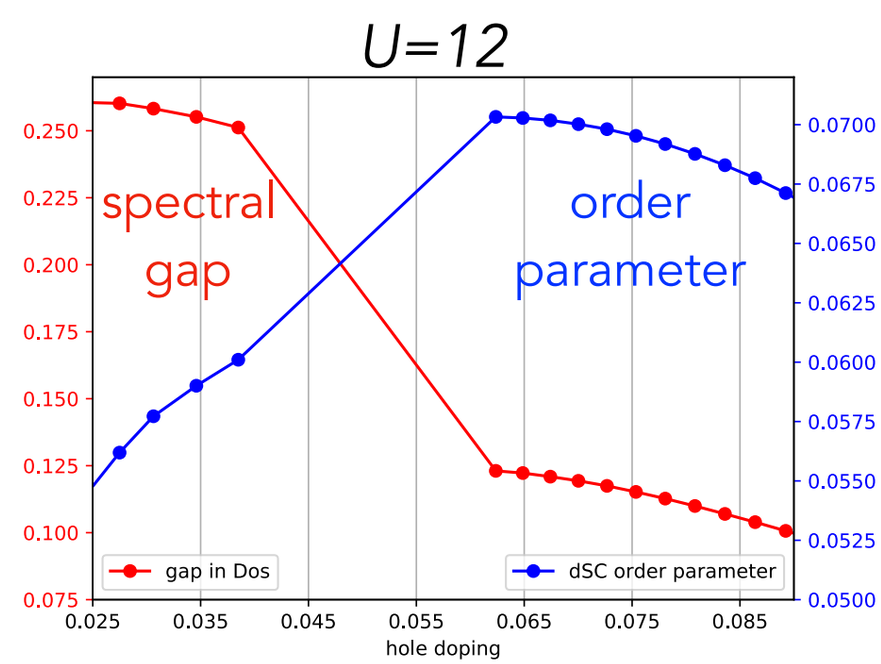




overdoped : the gap increases with the order parameter

underdoped : the gap jumps up (pseudogap) & the order parameter decreases



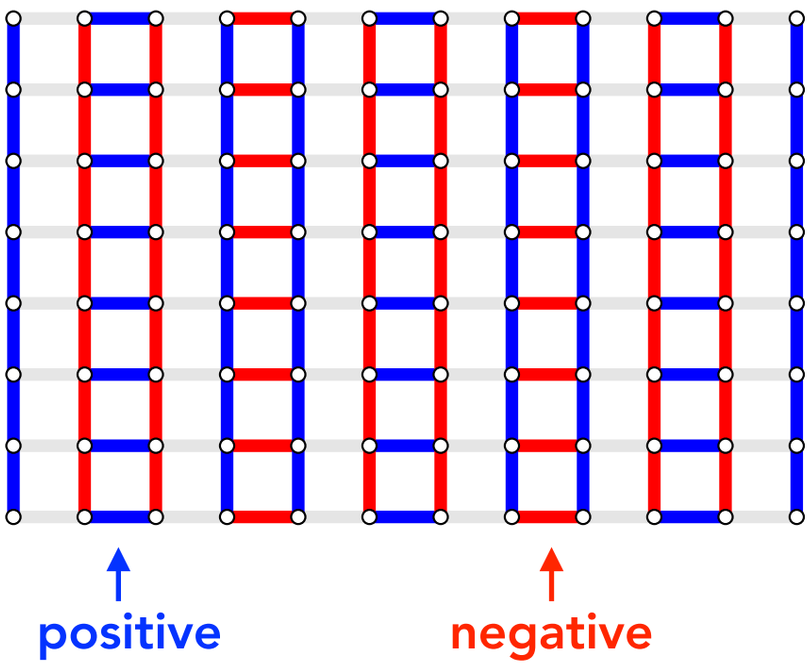


S. Dash & DS, in preparation

Charge order

for a review : Comin & Damascelli, Annu. Rev. Condens. Matter Phys. 2016. **7**:369

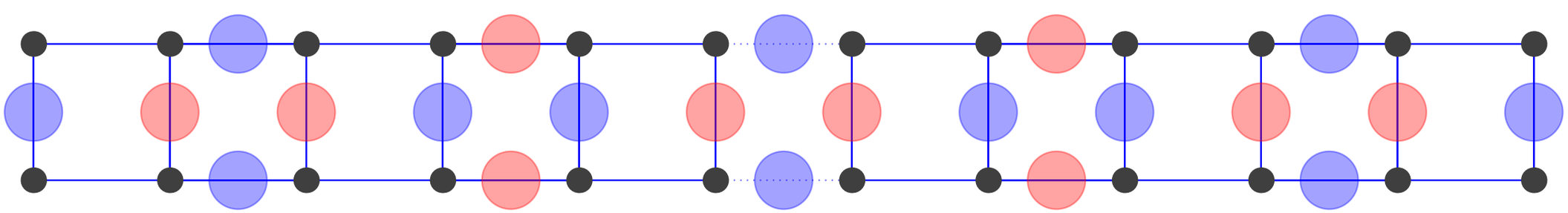
- Charge modulation located on the oxygen atoms
- In the 1-band model → bond density wave (BDW)



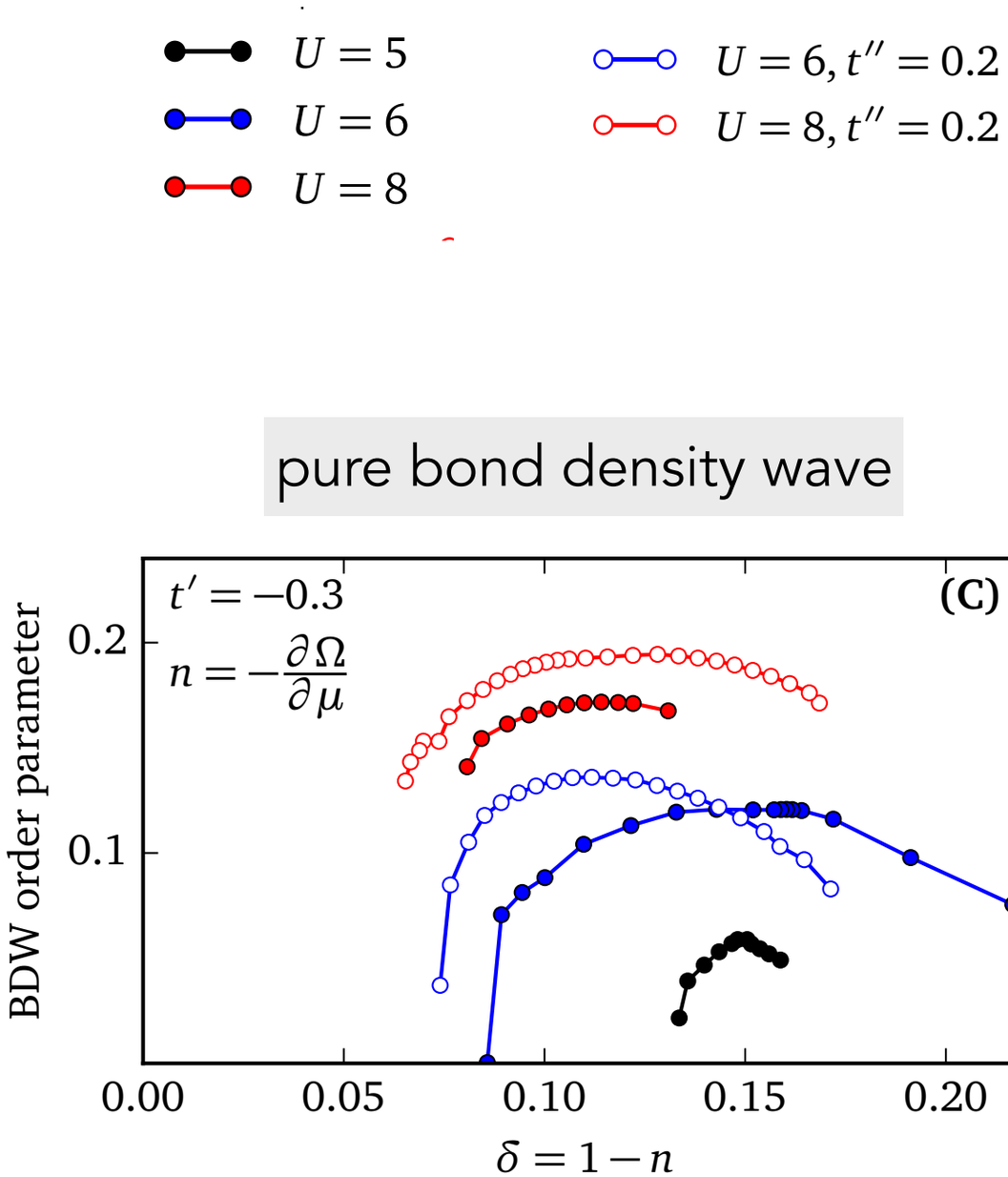
$$\hat{\Psi}_{\mathrm{BDW}} = \sum_{\mathbf{r}\sigma,\mathbf{a}} t_{\mathbf{q},\mathbf{a}} c^{\dagger}_{\mathbf{r},\sigma} c_{\mathbf{r}+\mathbf{a},\sigma} e^{i(\mathbf{q}\cdot\mathbf{r}+\mathbf{a}/2)} + \mathrm{H.c}$$

$$\hat{\Psi}_{\mathrm{PDW}} = \sum_{\mathbf{r},\mathbf{a}} t_{\mathbf{q},\mathbf{a}} (c_{\mathbf{r},\uparrow} c_{\mathbf{r}+\mathbf{a},\downarrow} - c_{\mathbf{r},\downarrow} c_{\mathbf{r}+\mathbf{a},\uparrow}) e^{i(\mathbf{q}\cdot\mathbf{r}+\mathbf{a}/2)} + \mathrm{H.c}$$

VCA clusters



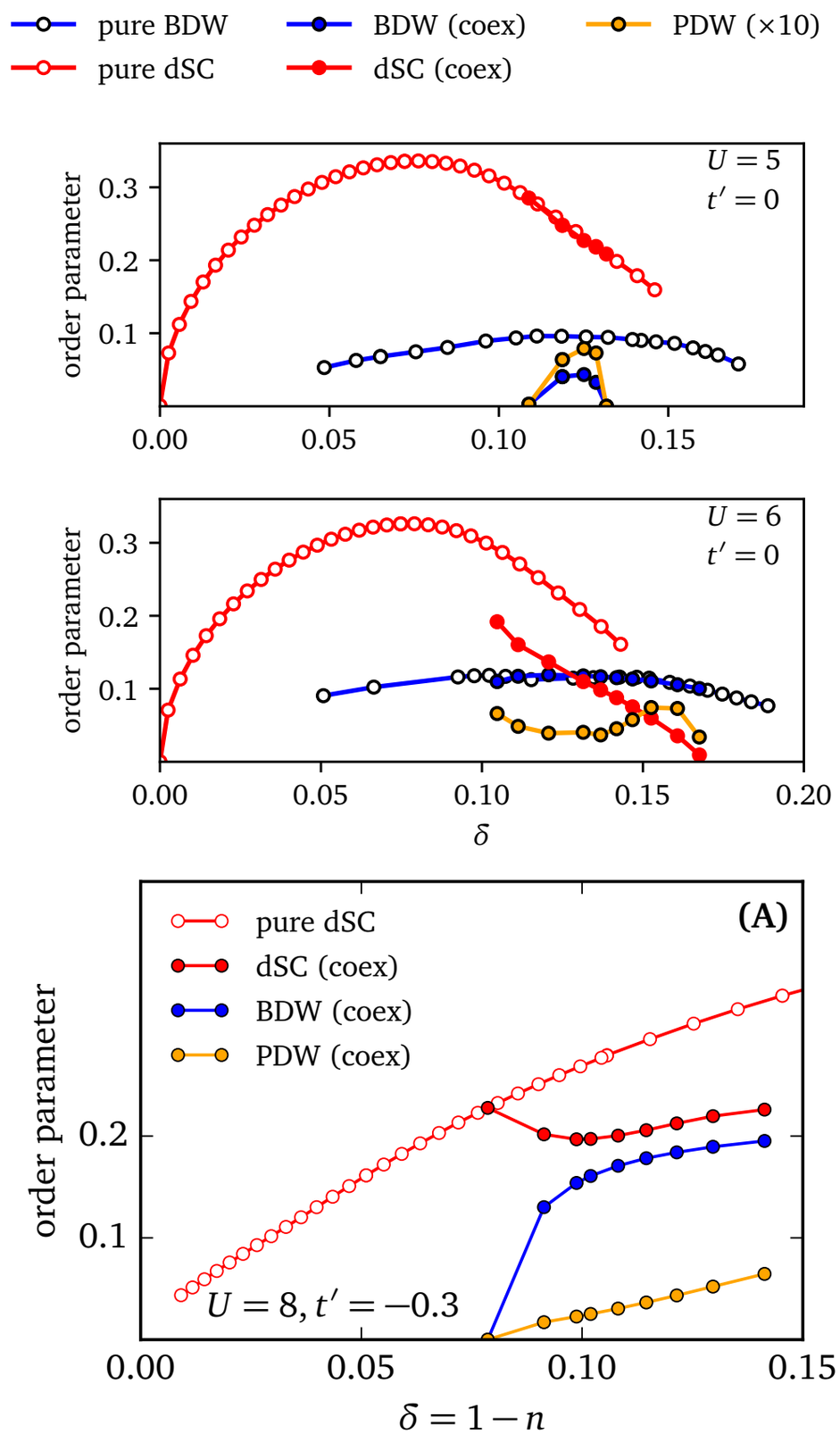
Charge order (VCA)



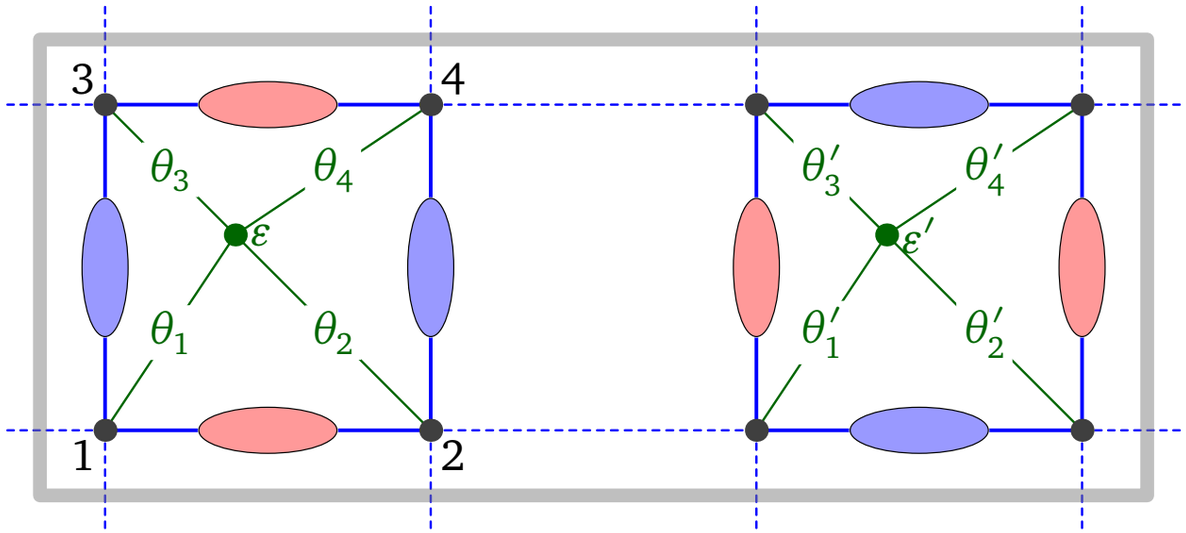
pure bond density wave

JPL Faye & DS, Phys. Rev. B **95** 115127 (2017)

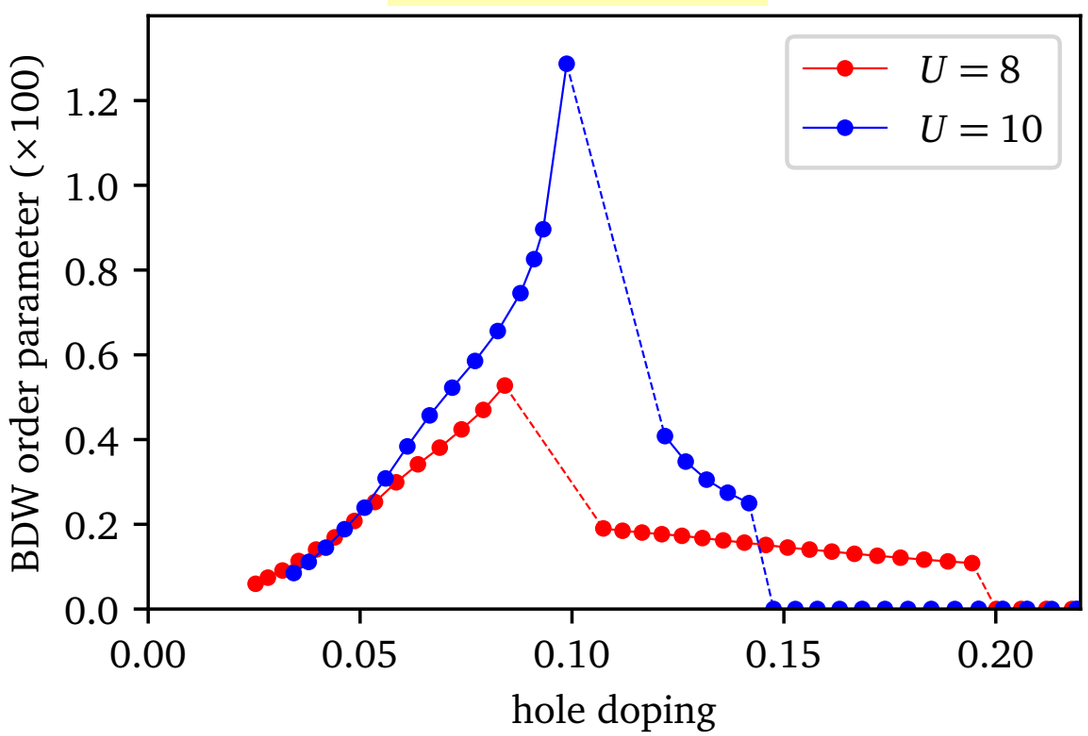
competition with d-wave superconductivity



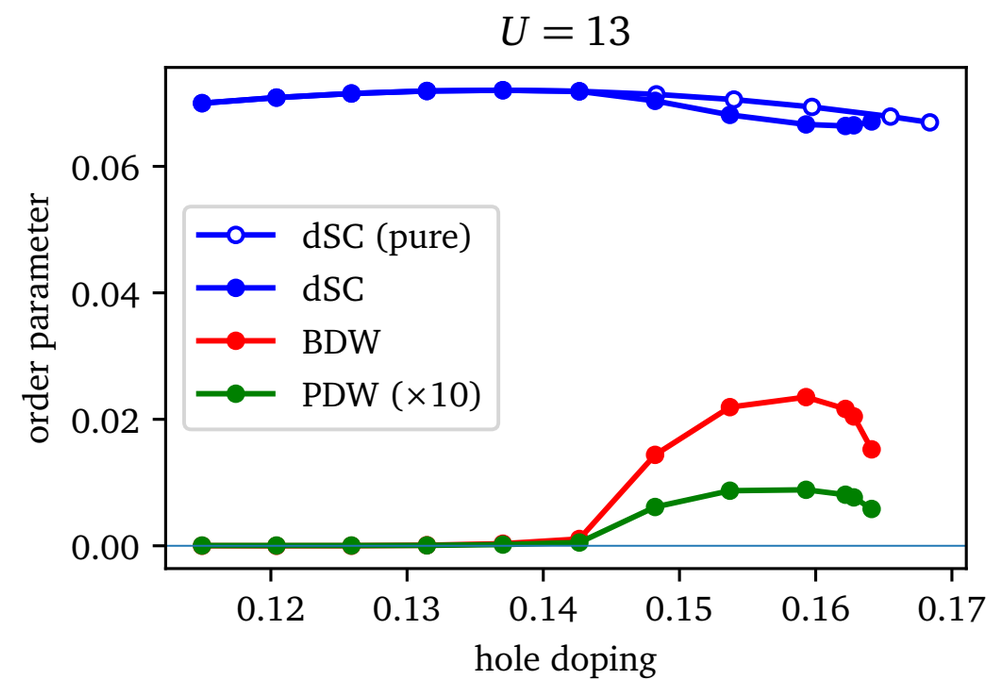
Charge order (CDMFT)

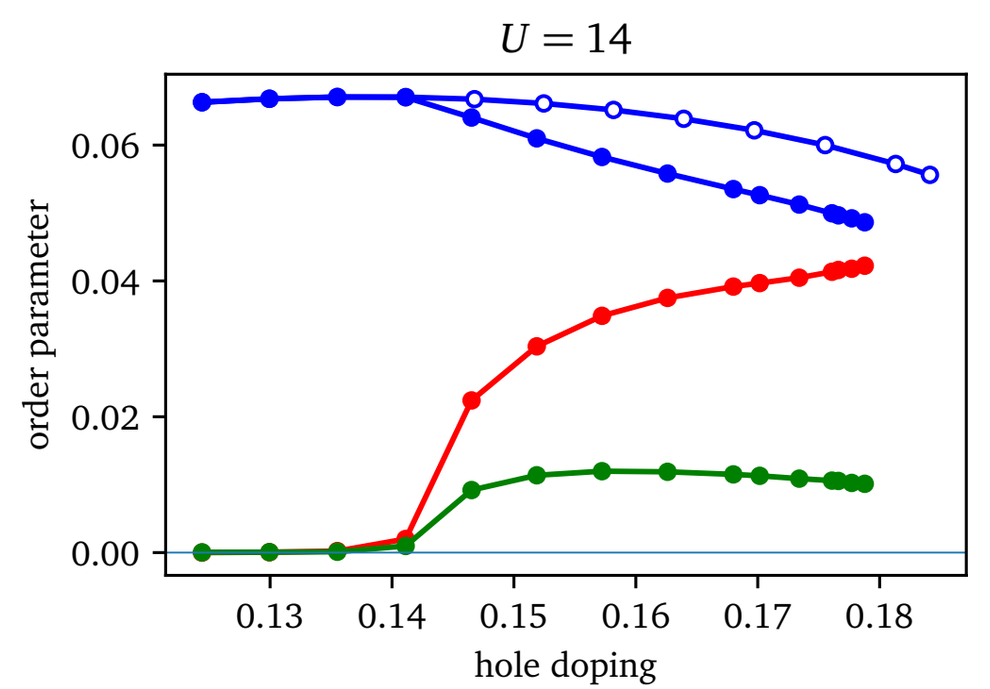


normal phase



with SC phase





S. Dash & DS, in preparation

loop currents

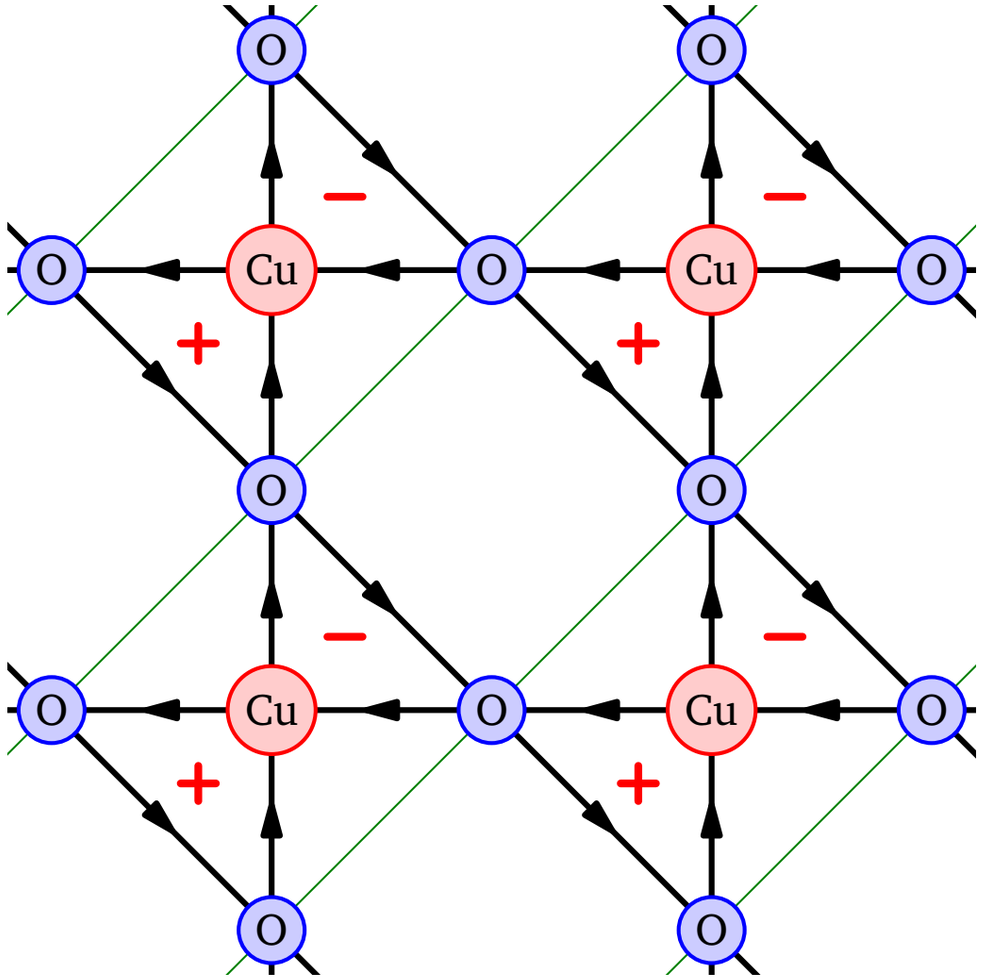
*Simon & Varma, PRL **89** 247003 (2002)*

current operator along direction **e** :

$$ic^{\dagger}_{\mathbf{r}}c_{\mathbf{r+e}} - ic^{\dagger}_{\mathbf{r+e}}c_{\mathbf{r}}$$

$$H \rightarrow H + I\hat{I}$$

Weiss field ⟵ ⟶ loop current operator



CDMFT strategy

- Allow complex-valued bath parameters
- Force the system by imposing nonzero I
- solve CDMFT repeatedly while decreasing I
- Measure order parameter $\langle\hat{I}\rangle$ vs I

Result : order parameter always zero. No loop current order !
But : single set of parameters. more work to be done…

Conclusions

- Superconductivity in strongly correlated materials can be studied using DMFT-like methods based on small clusters
- There are finite-size effects, and discrete bath effects, but the overall picture is consistent
- Competing orders can also be studied : AFM, charge order
- 1-band & 3-band models capture the physics of cuprates

Thank you!

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The Variational Cluster Approximation (VCA)

technical slide

- Add Weiss field(s) to the cluster
- Set their values by optimizing the Potthoff functional

G.S. energy of cluster

inter cluster hopping

$$\Omega(M) = \Omega'(M) - \int \frac{\mathrm{d}\omega}{\pi} \sum_{\tilde{\mathbf{k}}} \ln\det\left[1 - \mathbf{V}(\tilde{\mathbf{k}})\mathbf{G}(i\omega)\right]$$

Potthoff functional

cluster Green function

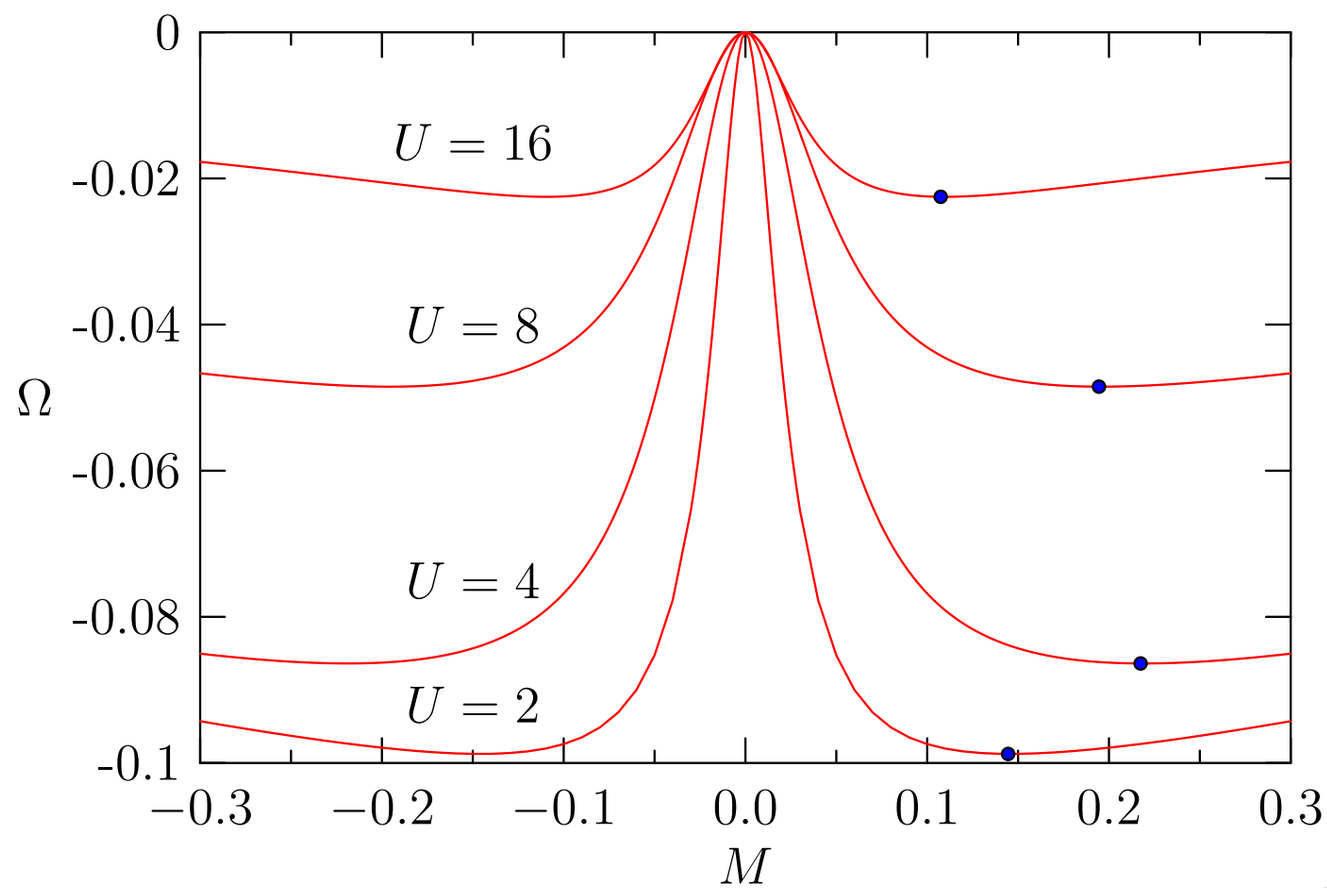
Example : Néel antiferromagnetism

Weiss field

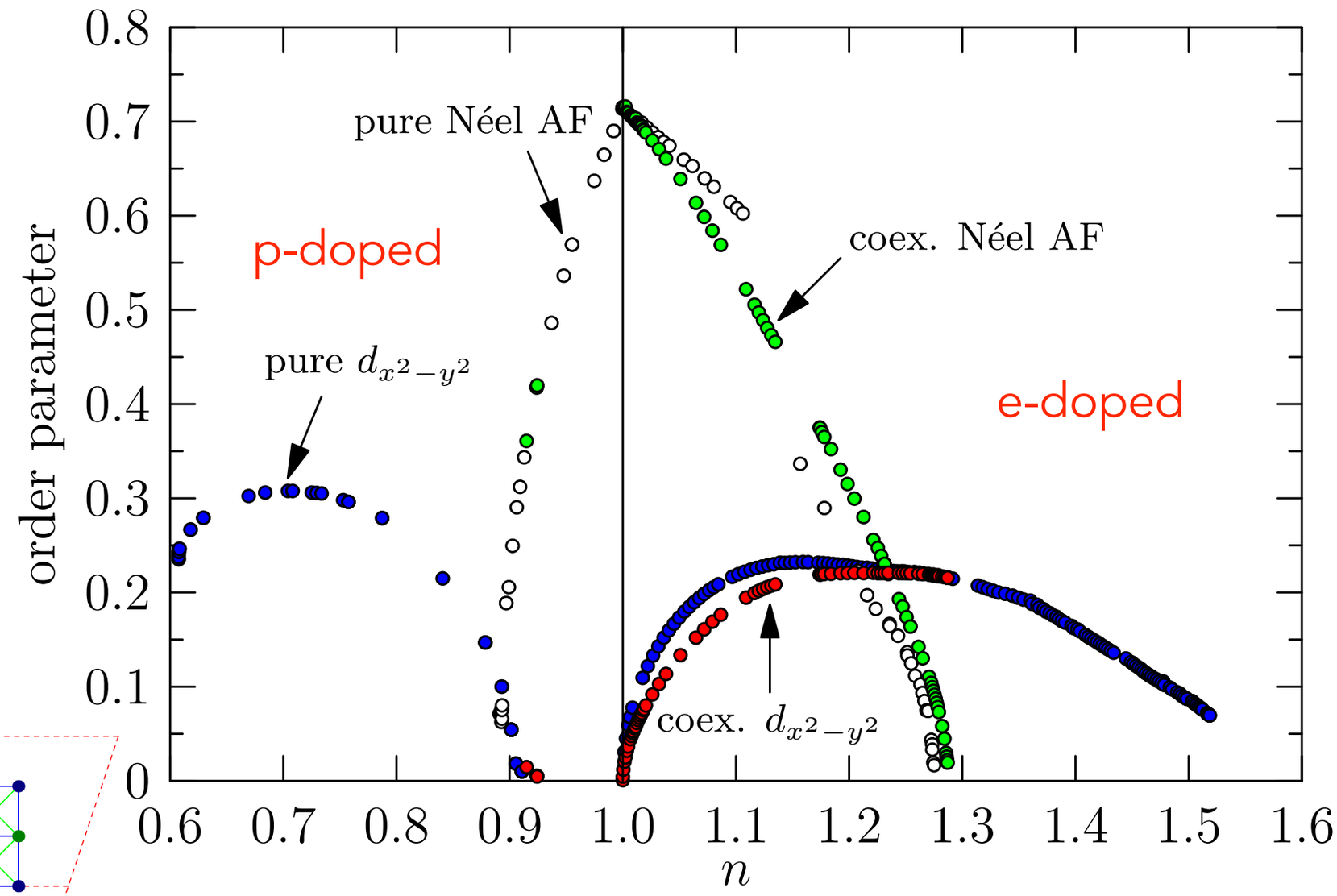
$$H_M = M\hat{M}$$

$$\hat{M} = \sum_{\mathbf{r}} e^{i\mathbf{Q}\cdot\mathbf{r}}\left(n_{\mathbf{r}\uparrow} - n_{\mathbf{r}\downarrow}\right)$$

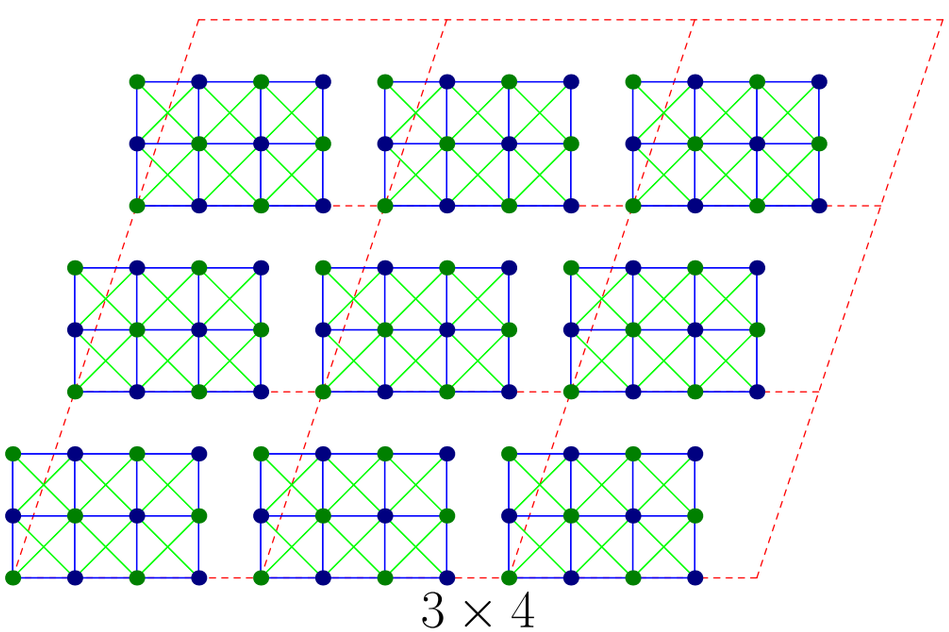
order parameter : $\langle \hat{M} \rangle / N_{\text{sites}}$



VCA : phase diagram for YBCO



12-site cluster

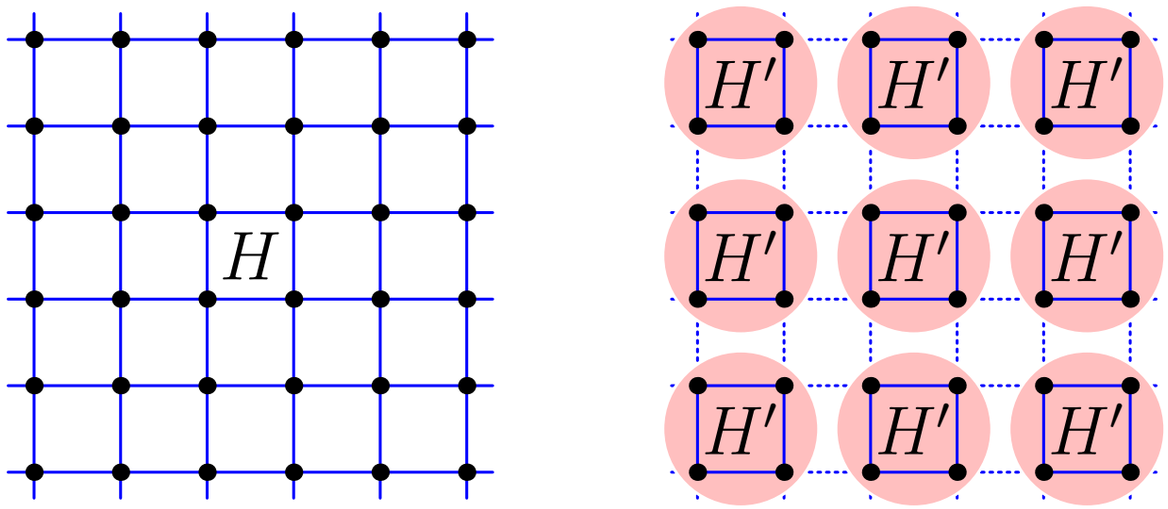


$$t = 1\ ,\ t' = -0.3\ ,\ t'' = 0.2$$

M. Guillot, MSc thesis, 2007

(Cluster) Dynamical Mean Field Theory

technical slide



- Environment of cluster replaced by uncorrelated « bath »
- Bath parameters determined by self-consistency relation

cluster Hamiltonian — hybridization — bath orbital

$$H' = \sum_{\alpha,\beta} t'_{\alpha\beta} c^\dagger_\alpha c_\beta + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{r,\alpha} \theta_{r\alpha} (c^\dagger_\alpha a_r + \text{H.c.}) + \sum_r \varepsilon_r a^\dagger_r a_r$$

bath energies

Green function :

$$\mathbf{G}'(i\omega_n)^{-1} = i\omega_n - \mathbf{t}' - \mathbf{\Gamma}(i\omega_n) - \mathbf{\Sigma}(i\omega_n)$$

Hybridization function :

$$\Gamma_{\alpha\beta}(i\omega_n) = \sum_r^{N_b} \frac{\theta_{\alpha r} \theta^*_{\beta r}}{i\omega_n - \varepsilon_r}$$

Adding superconductivity

technical slide

Adding a pairing term H_{pair} to the Hamiltonian :

VCA

$$H_{\text{pair}} = \sum_{\alpha,\beta} \Delta_{\alpha\beta} c_\alpha c_\beta + \text{H.c}$$

Nambu spinor : $\Psi_\alpha = \left(c_\alpha, c_\alpha^\dagger\right)$

one-body matrix:

$$\begin{pmatrix} \mathbf{t} & \Delta^\dagger \\ \Delta & -\mathbf{t}^* \end{pmatrix}$$

CDMFT

cluster ← → bath

$$H_{\text{pair}} = \sum_{\alpha,r} d_{\alpha r} c_\alpha a_r + \sum_{r,r'} \Delta_{r,r'} a_r a_{r'} + \text{H.c}$$

$$\Psi_\alpha = \left(c_\alpha, a_r, c_\alpha^\dagger, a_r^\dagger\right)$$

$$\begin{pmatrix} \mathbf{t} & \boldsymbol{\theta} & 0 & \mathbf{d}^\dagger \\ \boldsymbol{\theta}^\dagger & \boldsymbol{\varepsilon} & -\mathbf{d}^* & \Delta^\dagger \\ 0 & -\mathbf{d}^T & -\mathbf{t}^* & -\boldsymbol{\theta}^* \\ \mathbf{d} & \Delta & -\boldsymbol{\theta}^T & -\varepsilon^* \end{pmatrix}$$

The CDMFT self-consistency loop