Generating unconventional correlated electron systems through spontaneous charge ordering off half filling

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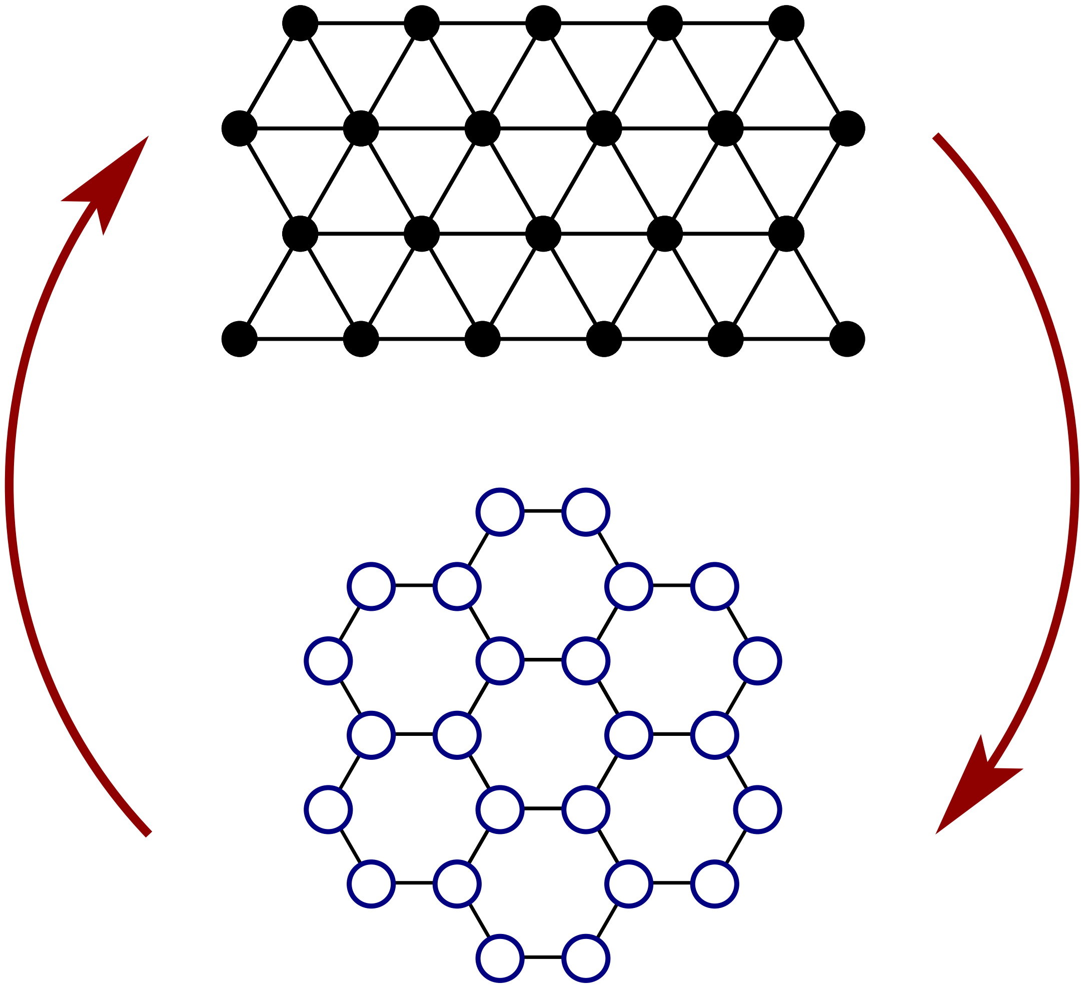
triangular ⇔ honeycomb



triangular lattice

n.n. kinetic energy

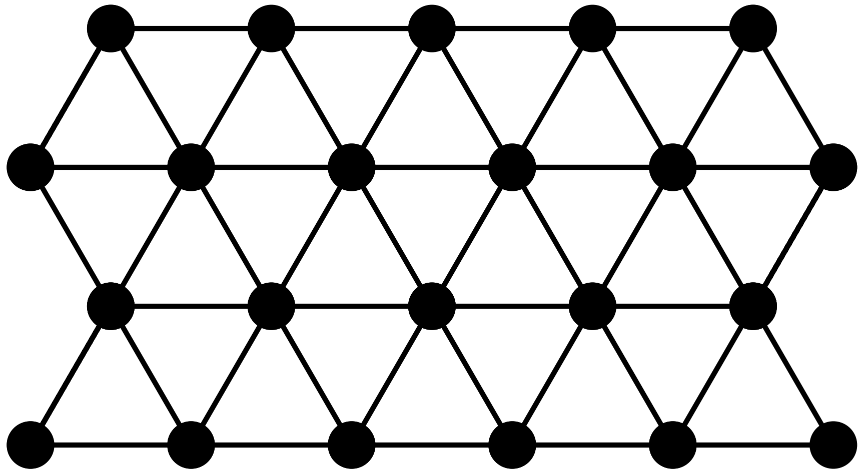
$$-t \sum_{<i,j>,\sigma} \left[c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right]$$

onsite Coulomb repulsion

$$U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

n.n. Coulomb repulsion

$$V \sum_{<i,j>} n_i n_j$$



* doping $\in [1/3, 1/2]$
* competition

  $t \Leftrightarrow U$

  $U \Leftrightarrow V$

variational Monte Carlo (VMC)

$$|\Psi\rangle = \mathcal{J}\mathcal{B}|\psi_0\rangle$$

$|\psi_0\rangle$: (generalized) Slater determinant

$\mathcal{J}$: diagonal density-density (spin-spin) Jastrow factor

$\mathcal{B}$: (non-diagonal) backflow corrections (not used here)

matrix elements

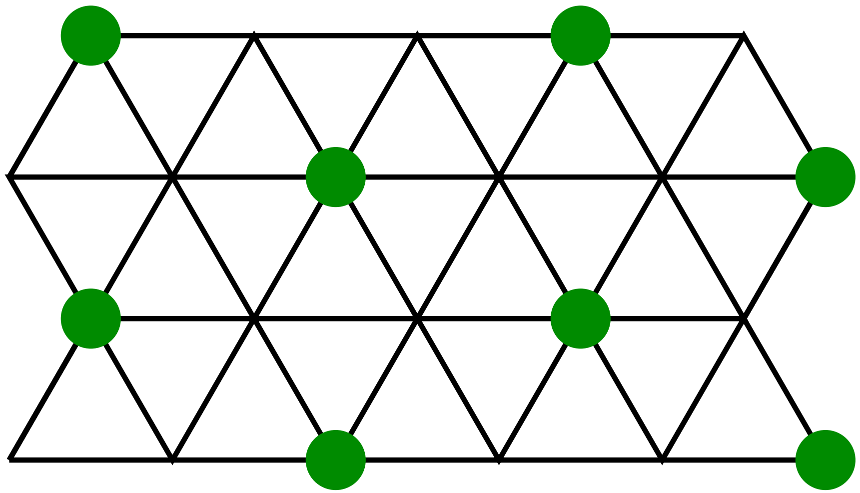
$$\frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_{\alpha,\beta}\langle\alpha|\hat{O}|\beta\rangle\frac{\langle\Psi|\alpha\rangle\langle\beta|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_{\alpha}\underbrace{\left(\sum_{\beta}\frac{\langle\alpha|\hat{O}|\beta\rangle\langle\beta|\psi\rangle}{\langle\alpha|\psi\rangle}\right)}_{f(\alpha)}\underbrace{\frac{|\langle\alpha|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle}}_{\rho(\alpha)}$$

Monte Carlo walk

weight : $\rho(\alpha)$

method : update of inverse determinants $\langle\alpha|\Psi\rangle$

charge ordered states



200 state

doping : $\delta = 1/3$

electrons : $\langle n_\uparrow + n_\downarrow \rangle = 2/3$

● : $|\uparrow\downarrow\rangle$

balance : $V > U$

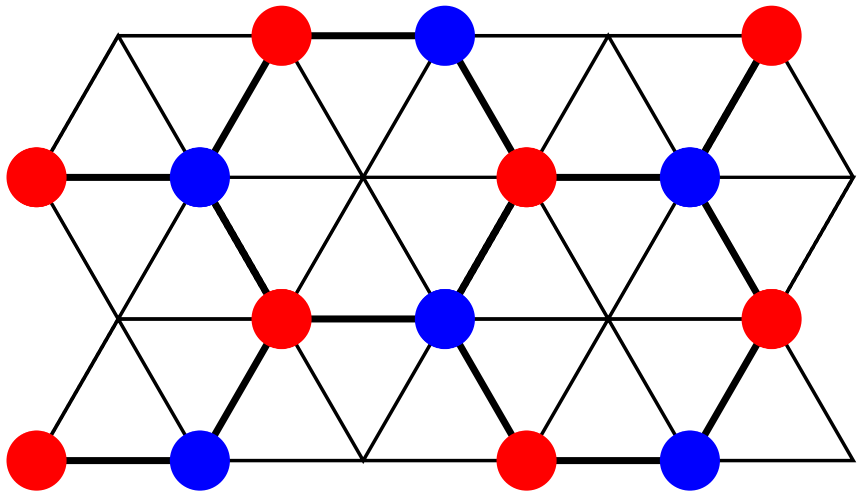
110 state

● : $|\uparrow\rangle$

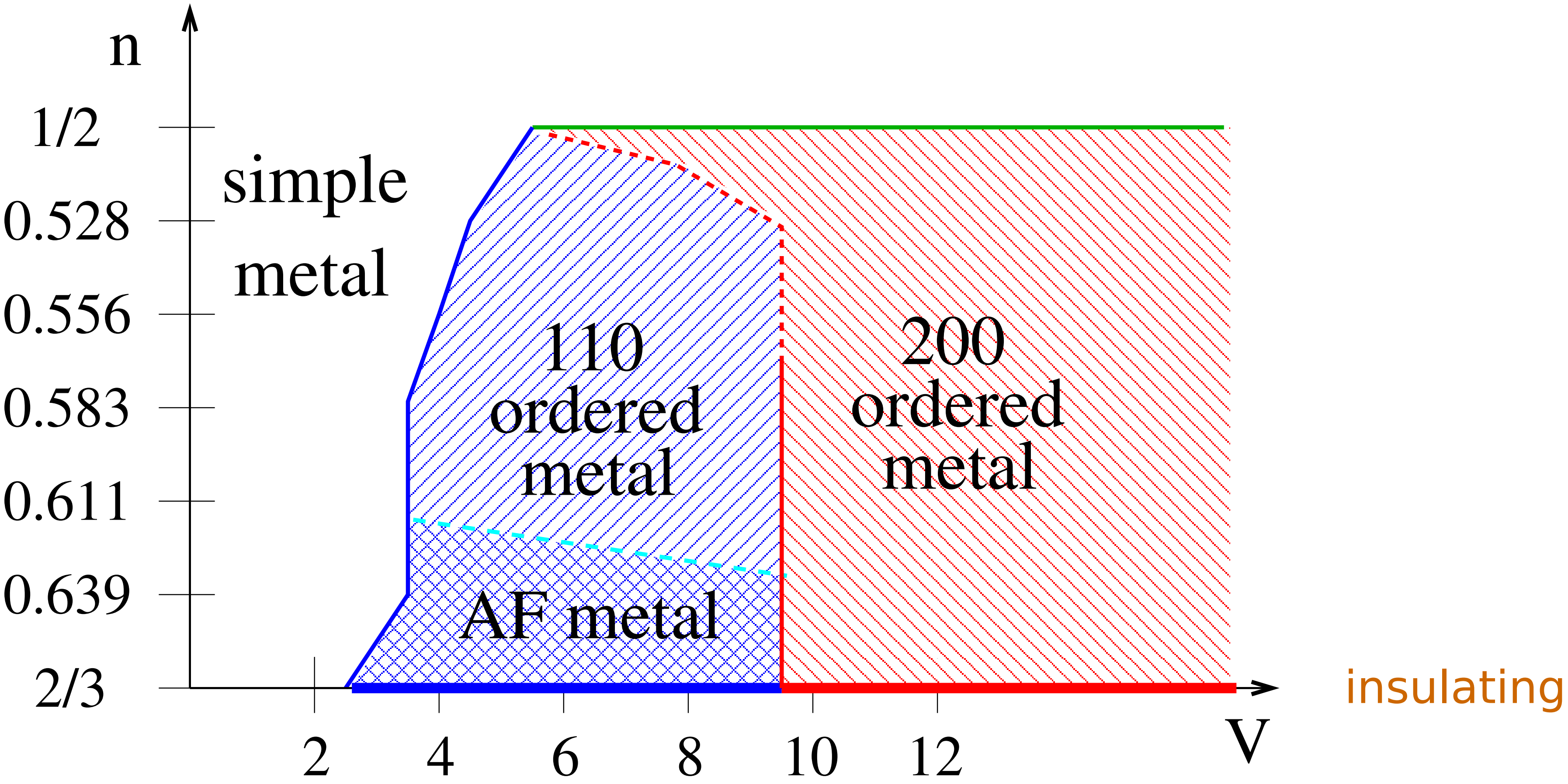
● : $|\downarrow\rangle$

balance : $U > V$

effective honeycomb



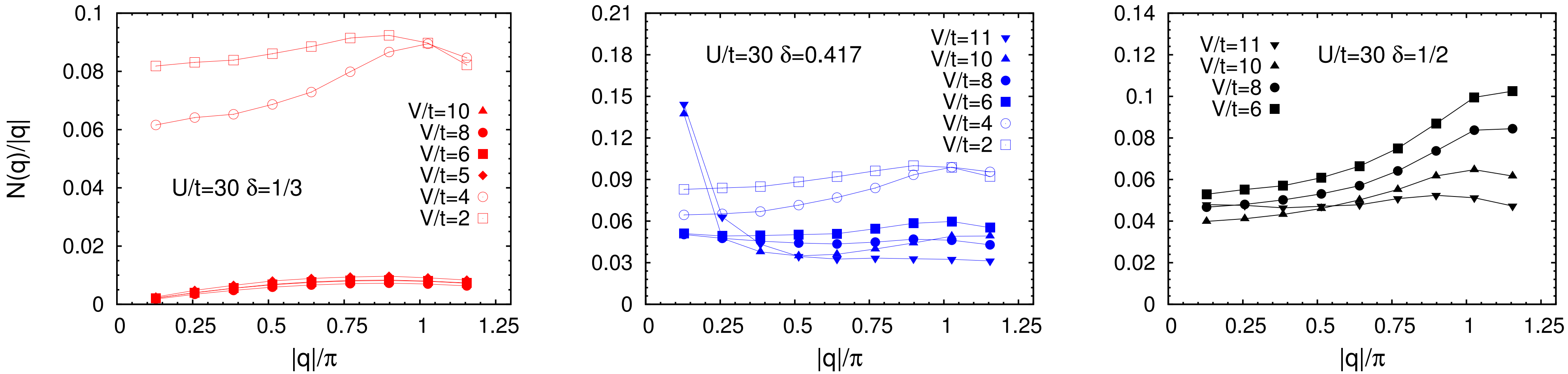
VMC phase diagram



[Tocchio, Feldner, Becca, Valenti, Gros, PRB ‘13]

Feynman charge density gap

$$|\Psi(q)\rangle = \sum_{\mathbf{R}} e^{\mathbf{R}\cdot\mathbf{q}} n_{\mathbf{R}} |\Psi\rangle \qquad E(q) \sim \frac{q^2}{N(q)} = \frac{q}{N(q)/q}$$

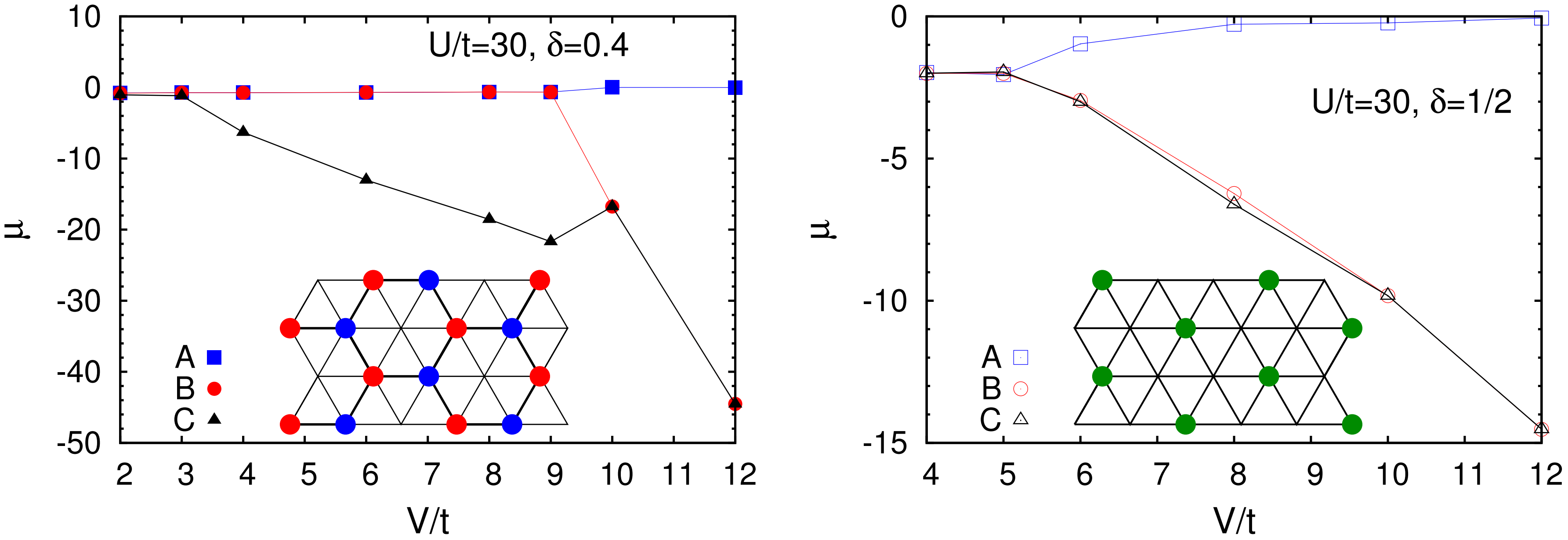


insulator : $\boxed{\dfrac{N(q)}{q} \sim q}$ $\qquad$ $\boxed{\dfrac{N(q)}{q} \sim \text{const.}}$: metal

local chemical potential

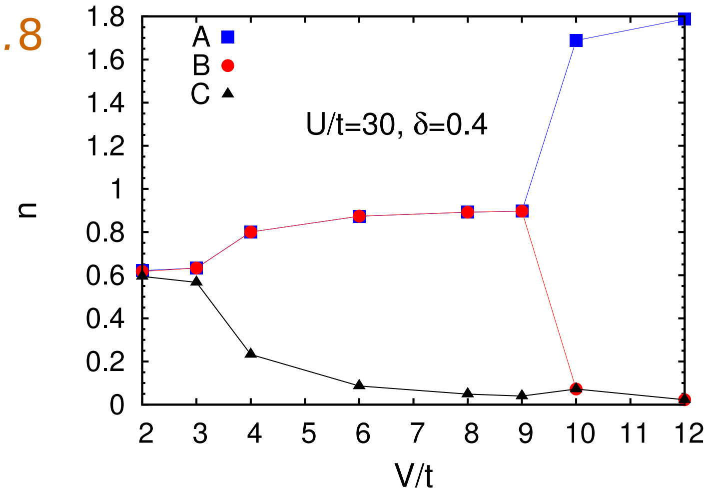
sublattice — variational parameters

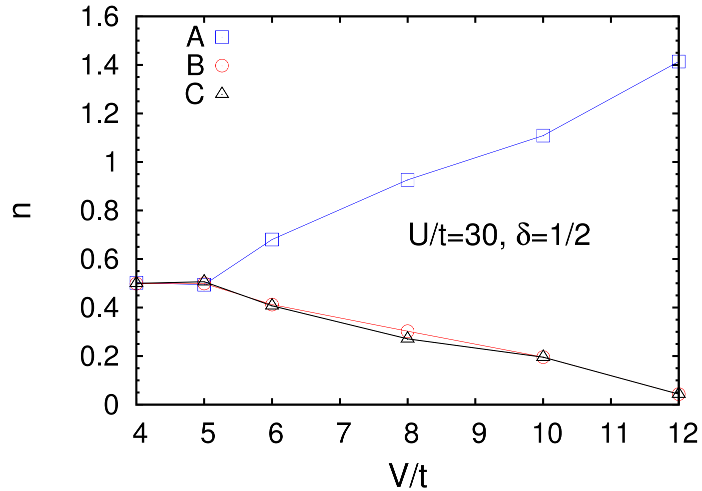
$$-\mu_A \sum_{\mathbf{R}\in A} n_{\mathbf{R}} - \mu_B \sum_{\mathbf{R}\in B} n_{\mathbf{R}} - \mu_C \sum_{\mathbf{R}\in C} n_{\mathbf{R}}$$



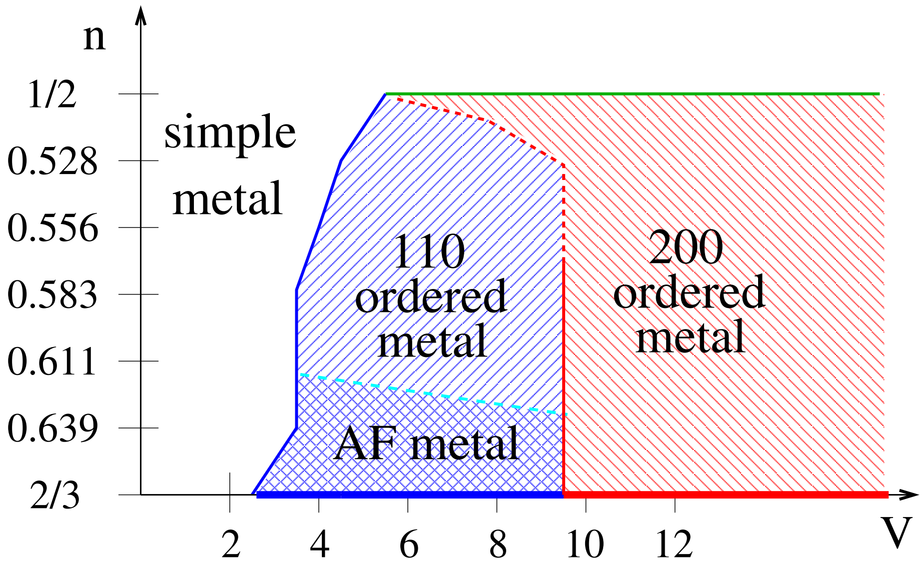
local site occupancy

$0.6 * 3 = 1.8$





$0.5 * 3 = 1.5$

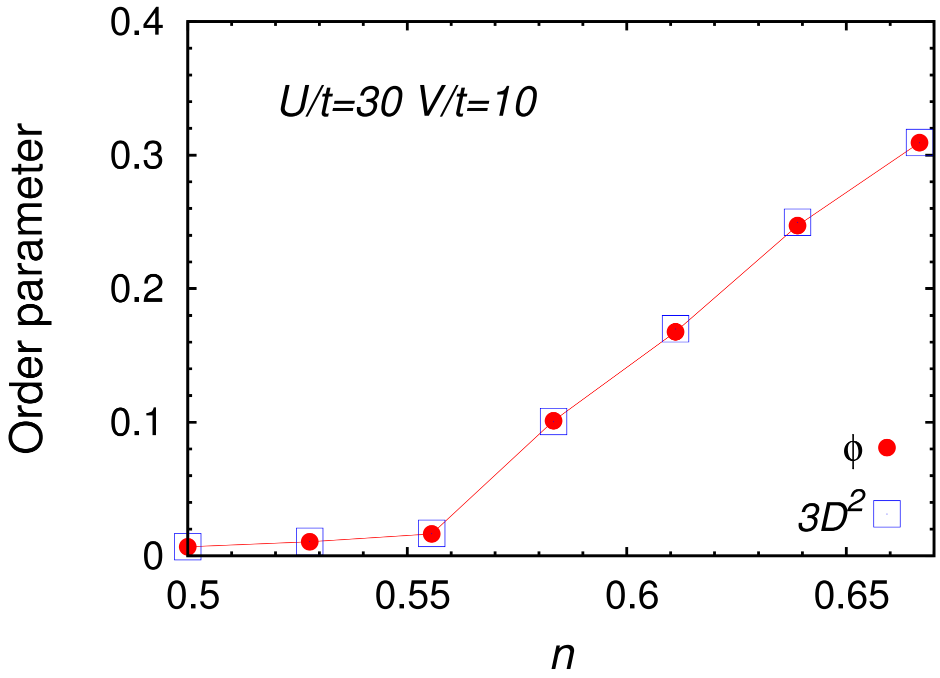


ordering of the 200 state

order parameter $\phi = \lim_{|i-j|\to\infty} \langle d_i d_j \rangle$ $d_i = n_{i,\uparrow} n_{i,\downarrow}$

distance $|i-j|$: A-A, B-B, C-C sublattices

doubly occupancy $D = \langle d_i \rangle$

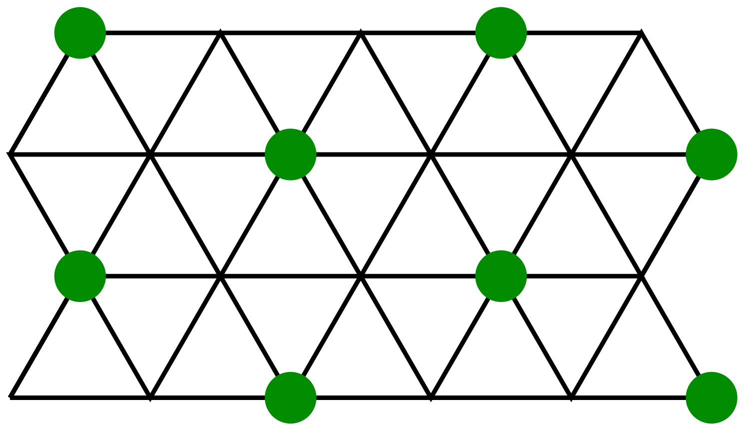


$\Phi = 3D^2$

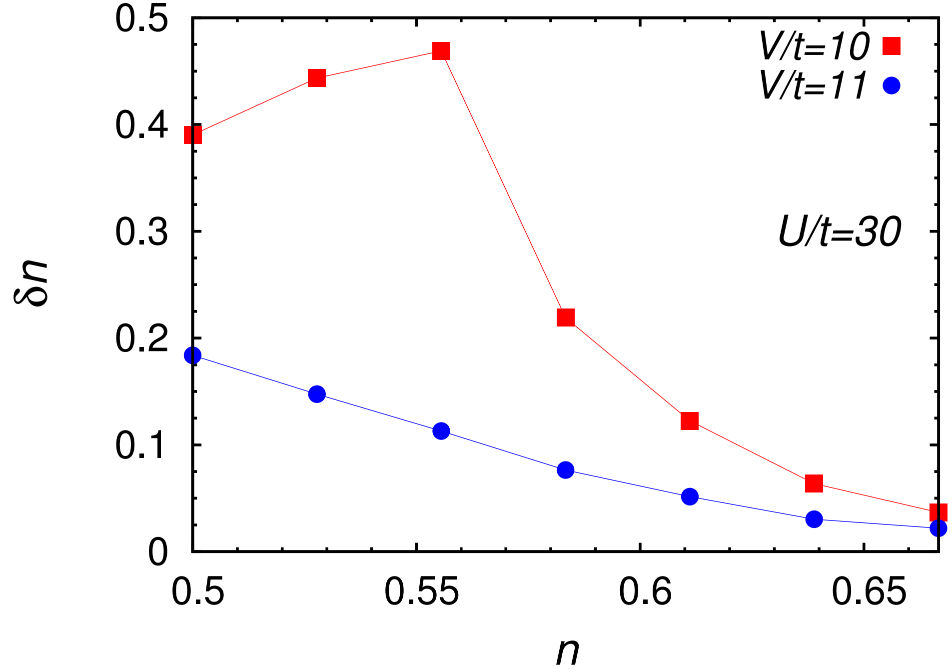
all doubly occupied sites contribute to charge ordering

no doubly occupied site contributes to charge transport

two fluid / pinball state



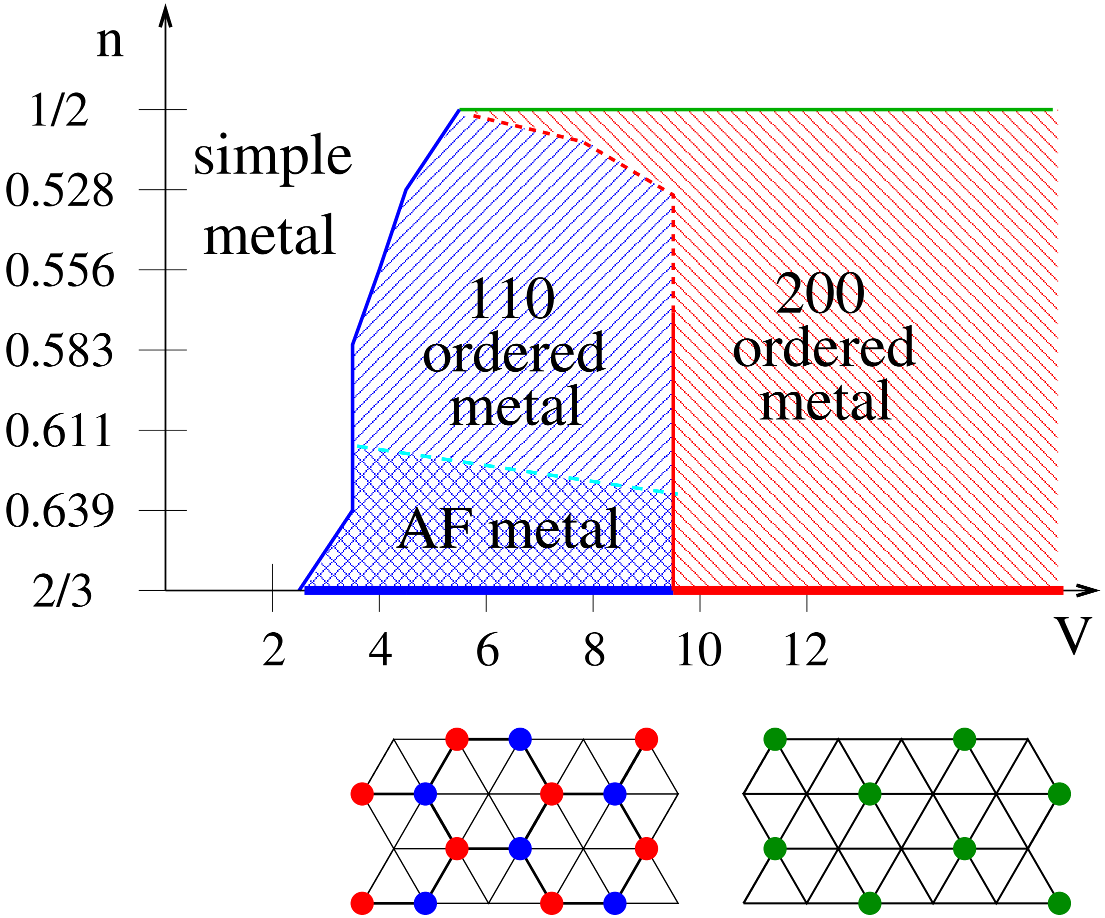
δn : occupancy of nearly empty sites



pinball state

[Hotta, Furukawa 2006/07]

metalic + commensurate charge order



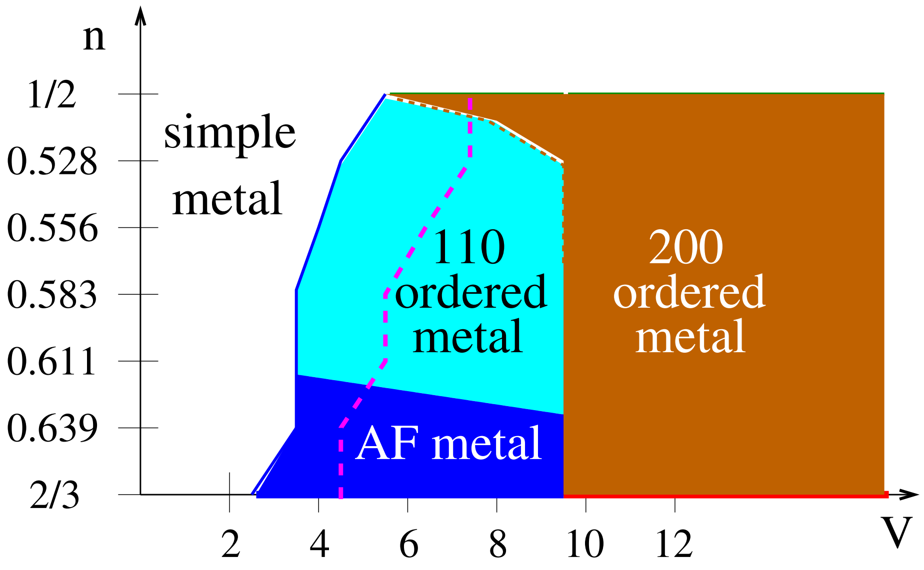
spontaneous symmetry breaking

.. through **translational invariant** wavefunctions

$$|\Psi\rangle \;=\; \mathcal{J}\,|\psi_0(\mu_A,\mu_B,\mu_C)\rangle \qquad\qquad \mathcal{J} \;=\; \exp\Big[-\textstyle\sum_{i,j} V_{|i-j|}n_i n_j/2\Big]$$

Jastrow factor $\quad \mathcal{J} \;:\; V_{|i-j|}$

Slater determinant $\quad |\psi_0(\mu_\alpha)\rangle \;:\;$ for $\;\mu_\alpha = 0$



dashed line:

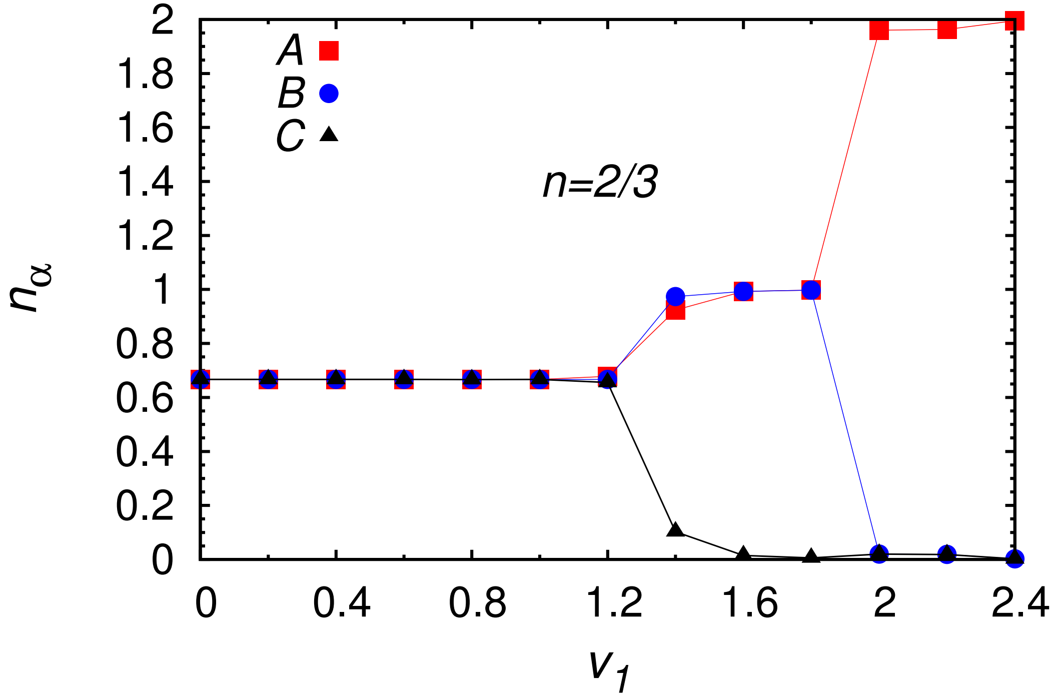
phase boundary for $\;\mu_\alpha = 0$

$|\Psi\rangle$ translational invariant

nearest neighbor Jastrow

$$|\Psi\rangle \ = \ \mathcal{J}\,|\psi_0(0)\rangle \qquad\qquad \mathcal{J} \ = \ e^{-g\sum_i n_{i,\uparrow} n_{j,\downarrow}}\, e^{-V_1 \sum_{<i,j>} n_i n_j/2}$$

no optimization: just a property of the wavefunction



$g = 5.0$

Monte Carlo sampling remains in a given broken symmetry state

(for long times)

statistical mechanics

.. of **energetically adapting** Jastrow factors

$$\left|\langle \mathbf{x}|\mathcal{J}|\psi_0\rangle\right|^2 \propto e^{-\beta H}$$

$$\beta H = V(\mathbf{x}) - \log(|\langle \mathbf{x}|\psi_0\rangle|^2)$$

$\mathbf{x}$: particle configuration: $\uparrow, \downarrow$: two-component ‘Coulomb’ gas

$V_{|i-j|}$: energetically optimized

$|\psi_0\rangle$: may contain variational parameters

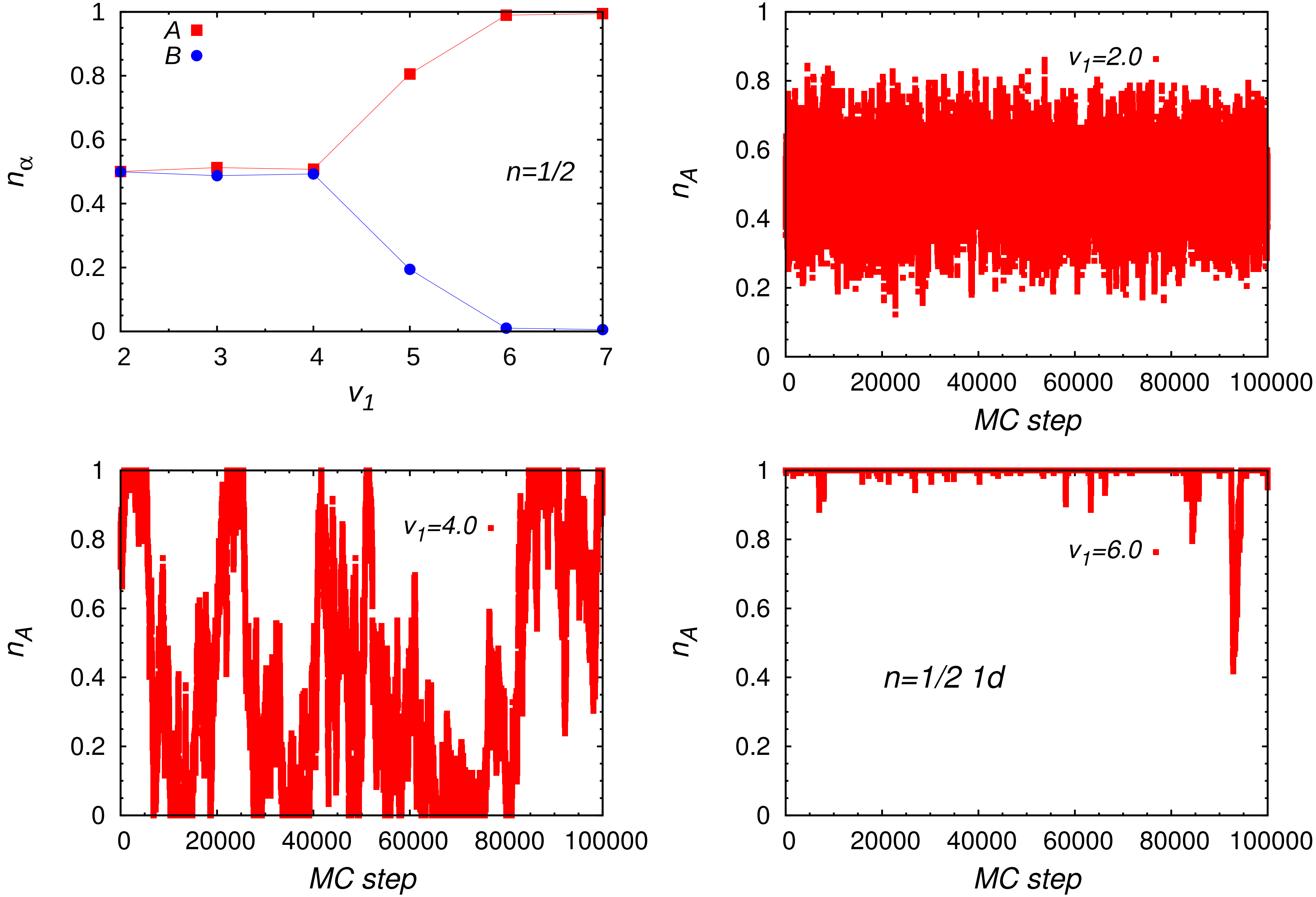
Variational Monte Carlo

searches for the ground state of a yet
to be determined ‘classical’ Hamiltonian

$\Longrightarrow$ spontaneous symmetry breaking

spontaneous ergodicity breaking

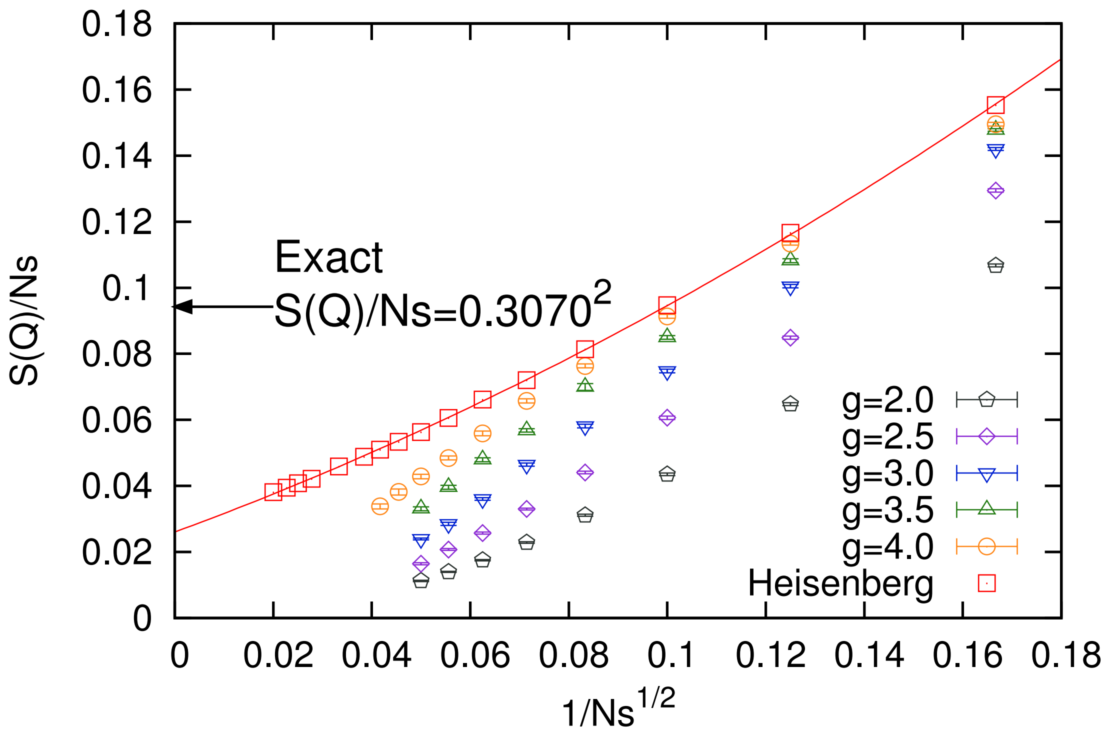
1D, $L = 244$, $n = 1/2$, $g = 10$



AF ordering of projected Fermi sea

2D square lattice, half filling

$$|\Psi\rangle = exp\left(-g\sum_i n_{i,\uparrow}n_{i,\downarrow}\right)|\psi_0\rangle \qquad |\psi_0\rangle = \prod_{k<k_F,\sigma} c^\dagger_{k,\sigma}|0\rangle$$



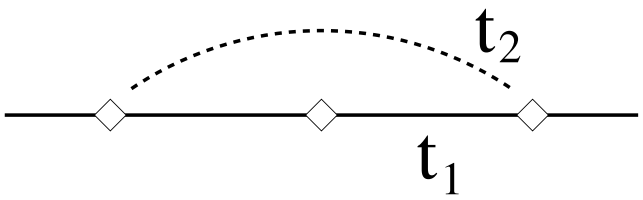
(only) fully projected Fermi sea AF ordered

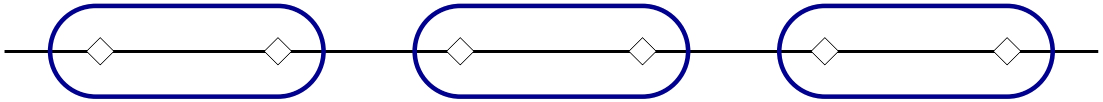
new data : $g < \infty$
Heisenberg : $g \to \infty$

[Tao Li, EPL '13]

» projecting out charge fluctuations enhances magnetic correlations «

spontaneous dimerization in 1D

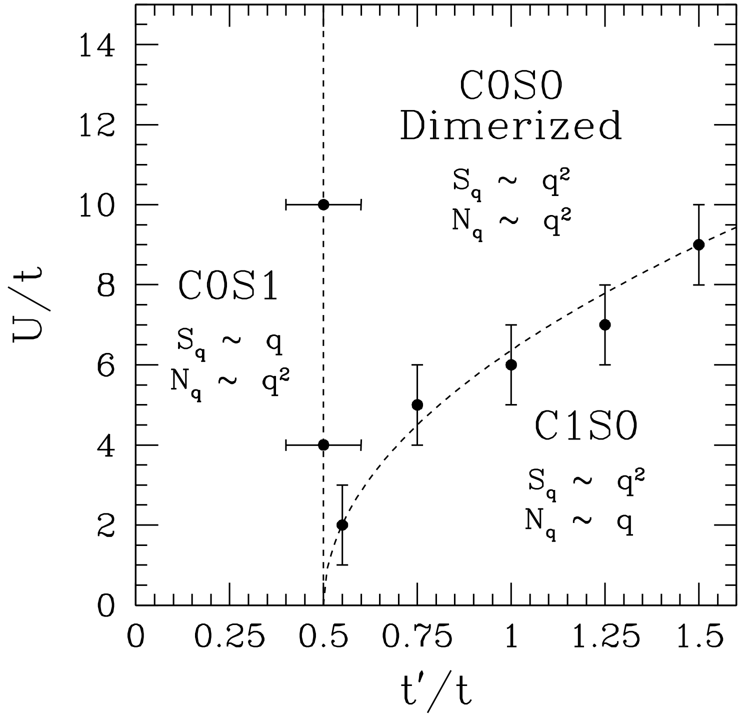




1D $t_1 - t_2 - U$ model

valence bond solid

[Capello, Becca, Fabrizio, Sorella, Tosatti, PRL '05]



spontaneous singlet ordering

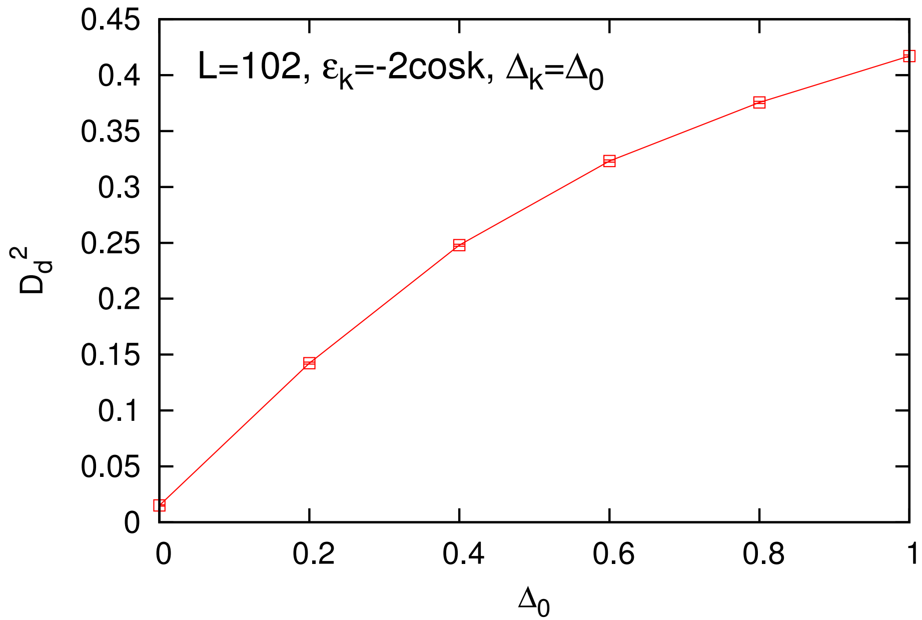
$$\frac{1}{\sqrt{2}}\left(c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow} + c^\dagger_{j,\uparrow}c^\dagger_{i,\downarrow}\right)$$

via translational invariant
variational wavefunctions

dimerized BCS wavefunction

$$|\Psi\rangle \;=\; e^{-g\sum_i n_{i,\uparrow}n_{i,\downarrow}}|\psi_{BCS}\rangle \qquad |\psi_{BCS}\rangle = \prod_k \left(u_k + v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}\right)|0\rangle$$

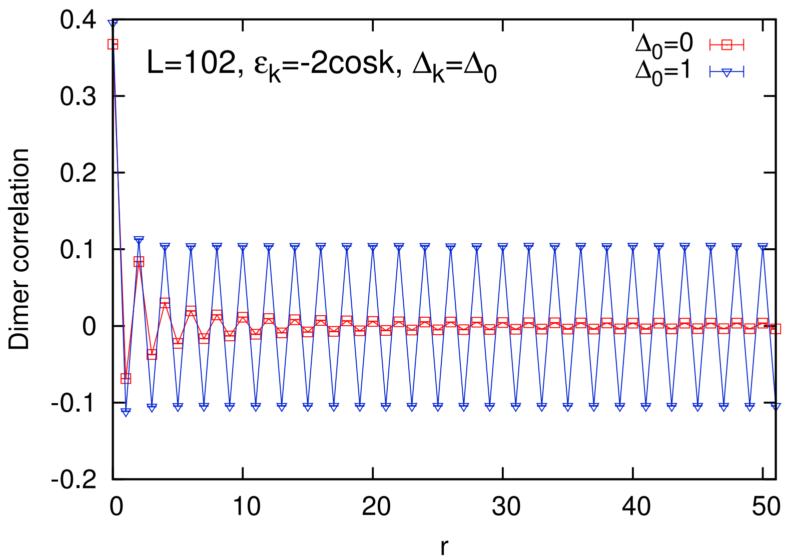
$$u_k^2/v_k^2 \;=\; \frac{1}{2}\left(1 \pm \frac{\epsilon_k}{\sqrt{\epsilon_k^2+\Delta_k^2}}\right)$$

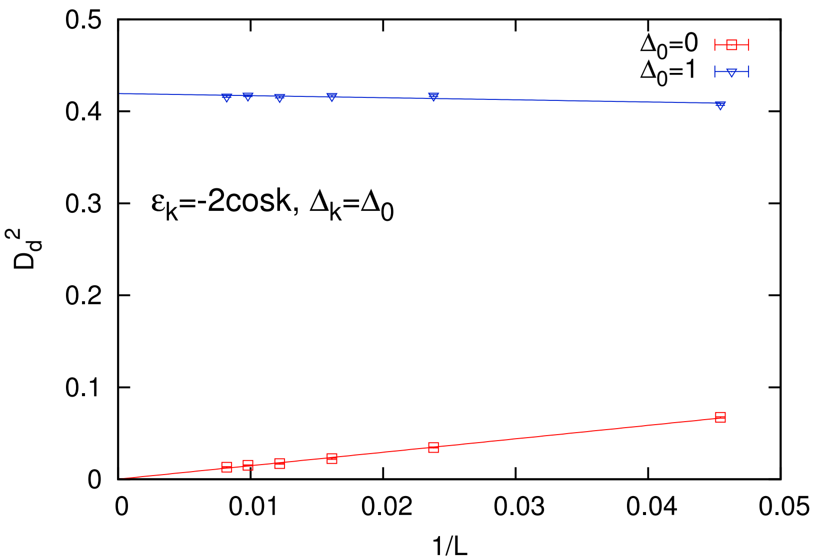


projecting out
particle number fluctuations
⇓
spontaneous dimerization

dimer ordering in 1D

$$Chi(r) = \frac{9}{L}\sum_i \left\langle \left(S_i^z S_{i+1}^z\right)\left(S_{i+r}^z S_{i+1+r}^z\right)\right\rangle - \left(\frac{3}{L}\sum_i \left\langle S_i^z S_{i+1}^z \right\rangle\right)^2$$



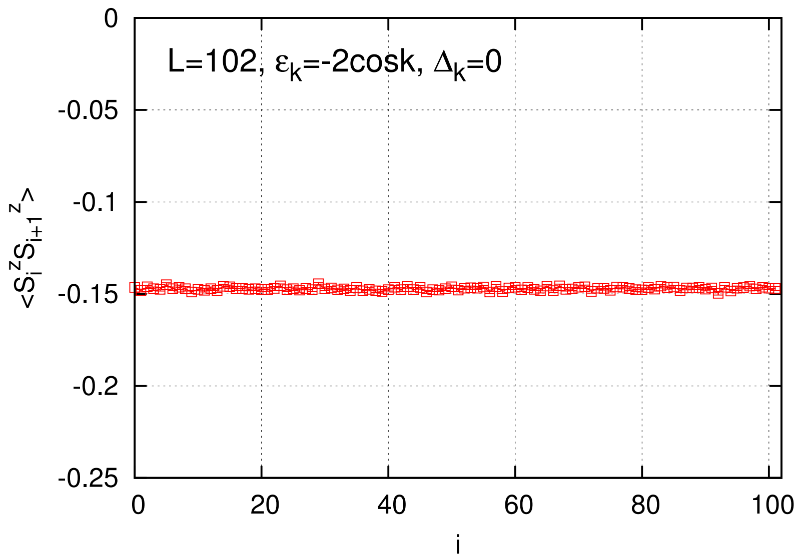


$$D_d^2 = lim_{r\to\infty}\left|2Chi(r) - Chi(r+1) - Chi(r-1)\right|$$

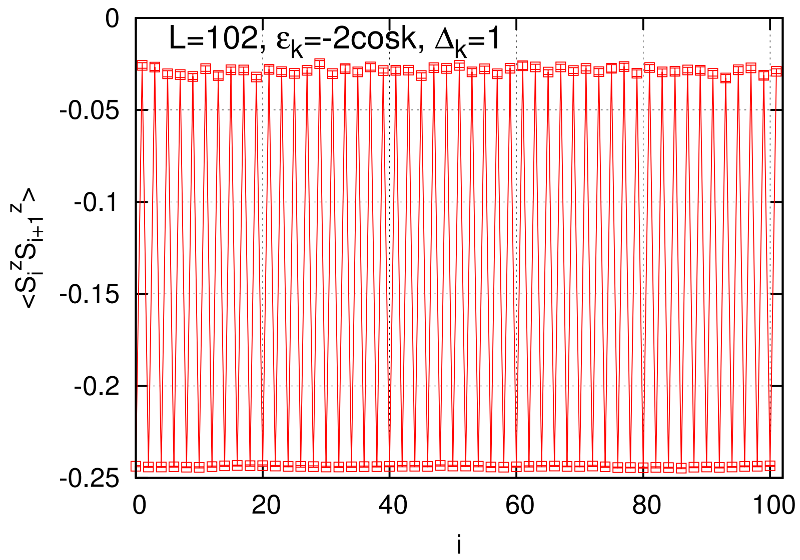
adiabaticity breaking

n.n. spin correlations in projected 1D states

Slater determinant



BCS wavefunction

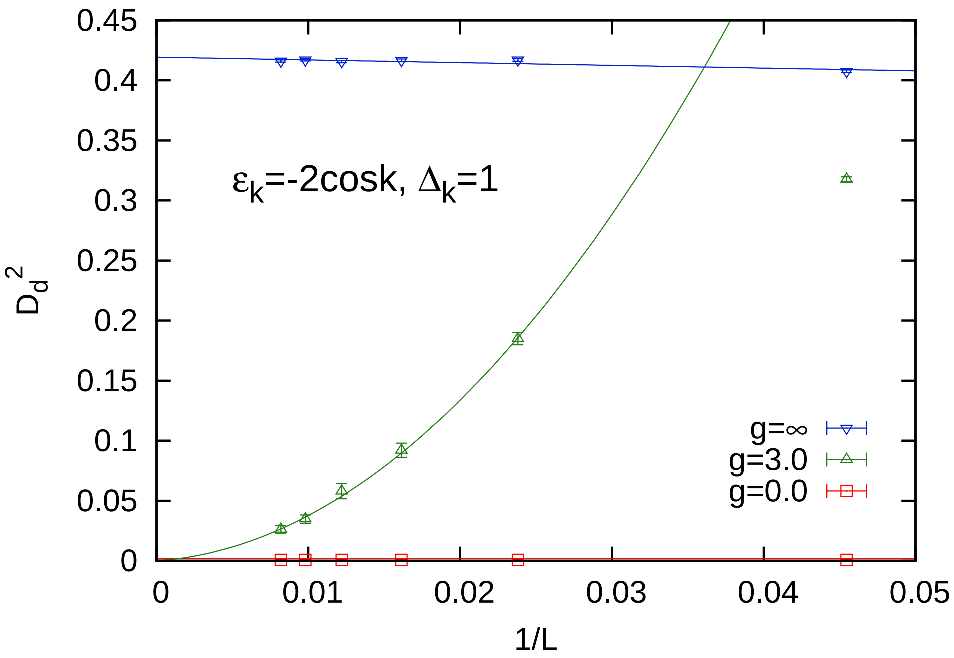


$$P_N|\psi_{BCS}\rangle = \prod_k \left(a_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}\right)^{N/2} |0\rangle \qquad a_k \propto v_k/u_k$$

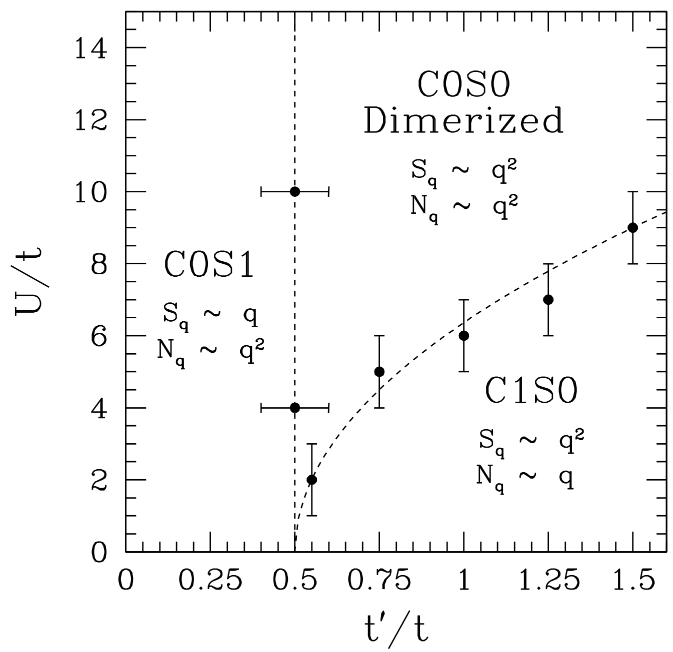
ordering vs. conduction

$$e^{-g\sum_i n_{i,\uparrow}n_{j,\downarrow}}\, e^{-\sum_{i\neq j} V_{|i-j|}n_i n_j/2} \prod_k \left(a_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}\right)^{N/2} |0\rangle$$

onsite only



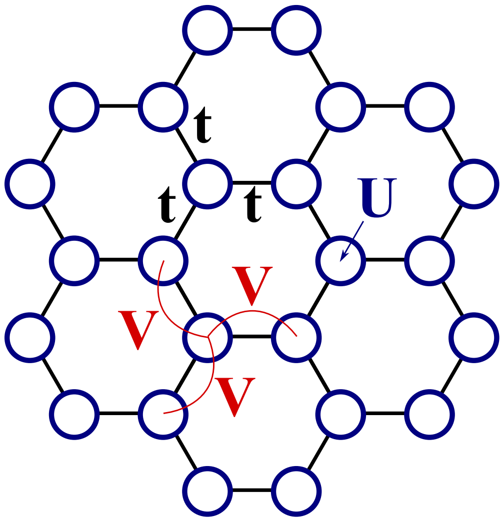
long-ranged Jastrow



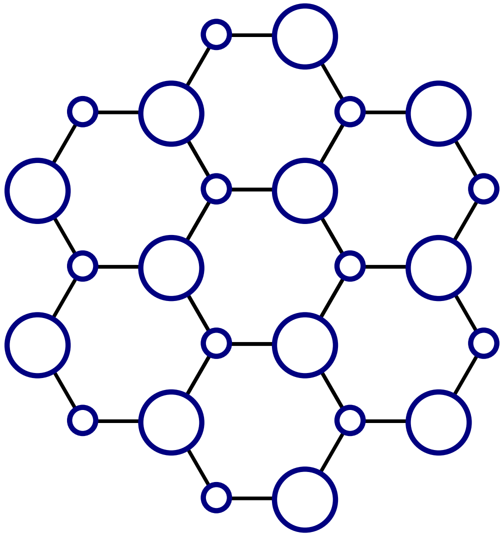
long-ranged Jastrow ⟹ insulating state
spontaneous dimer ordering ?

honeycomb lattice

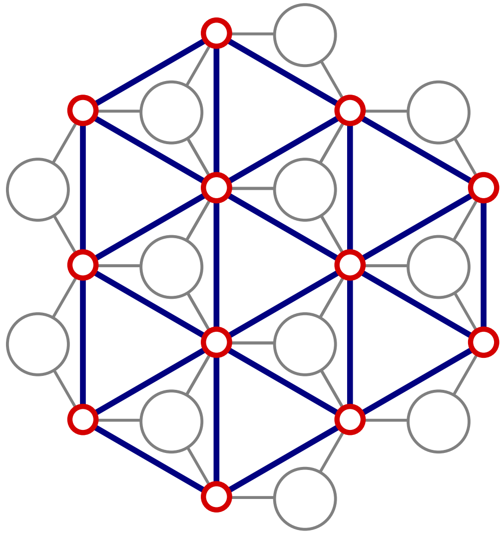
$t - U - V$ model



charge ordering



effective
triangular latttice



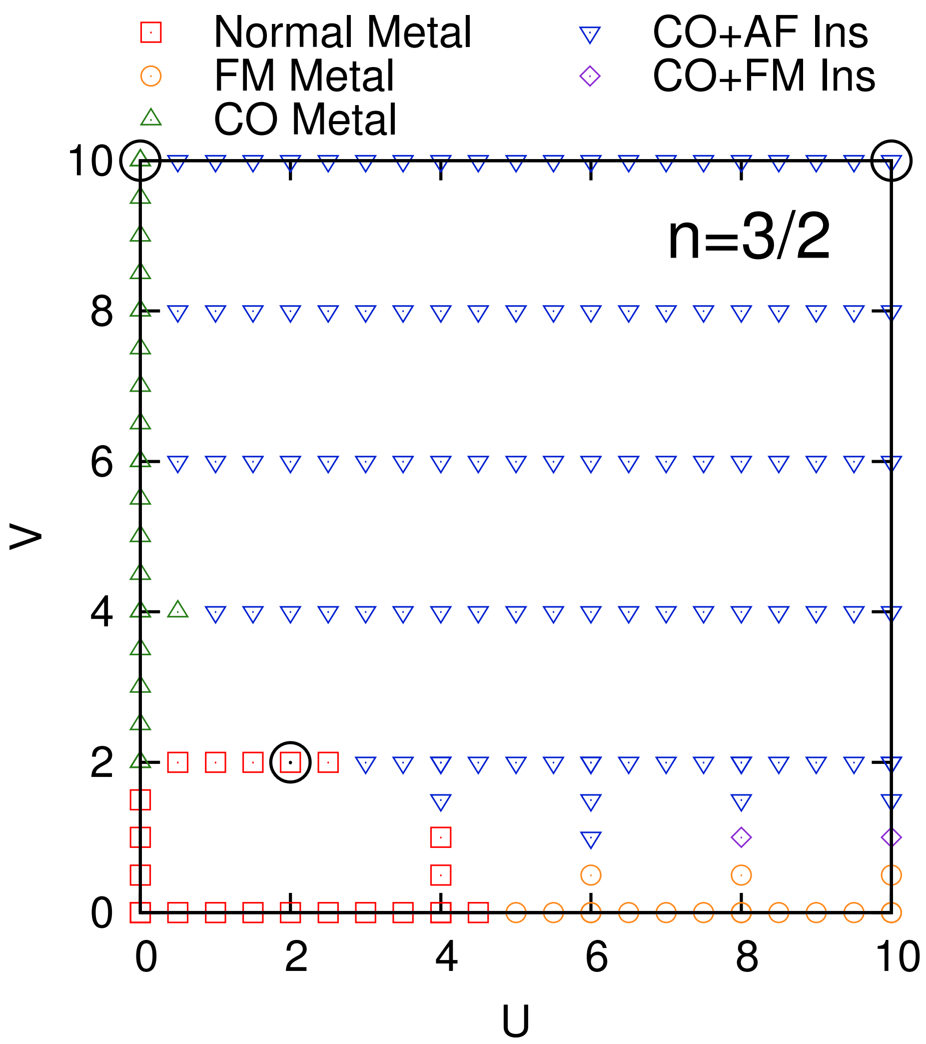
unconventional
couplings?

○ : singly occupied

◯ : doubly occupied

filling : 3/2 (motivated by charge-transfer salts)

honeycomb - mean field

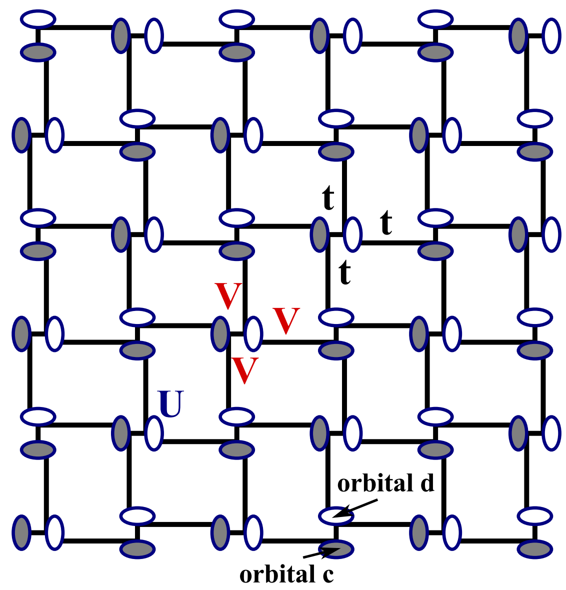


CO : charge-ordered

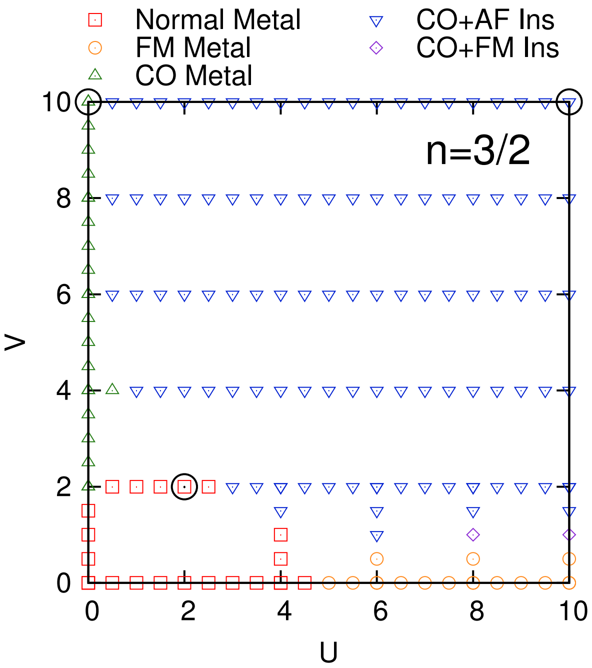
AM : antiferro-magnetic

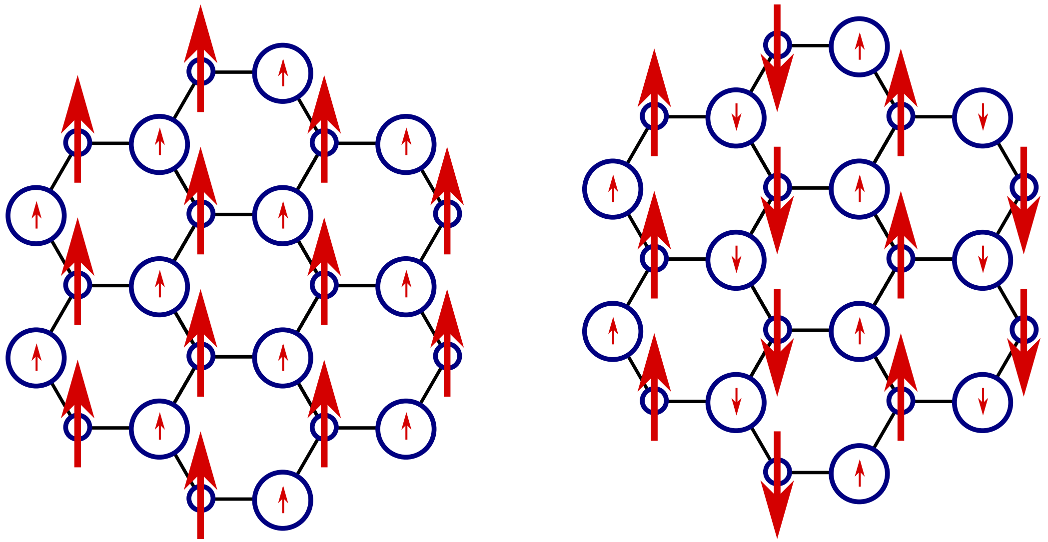
FM : ferro-magnetic

○ : VMC study



mean field states





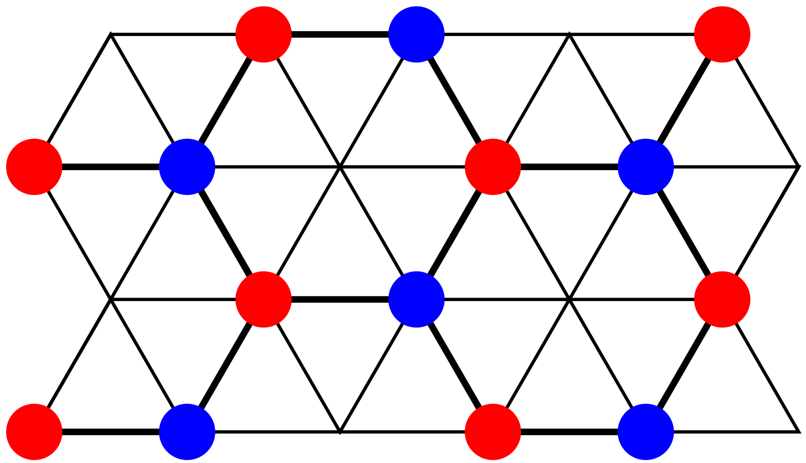
CO + FM

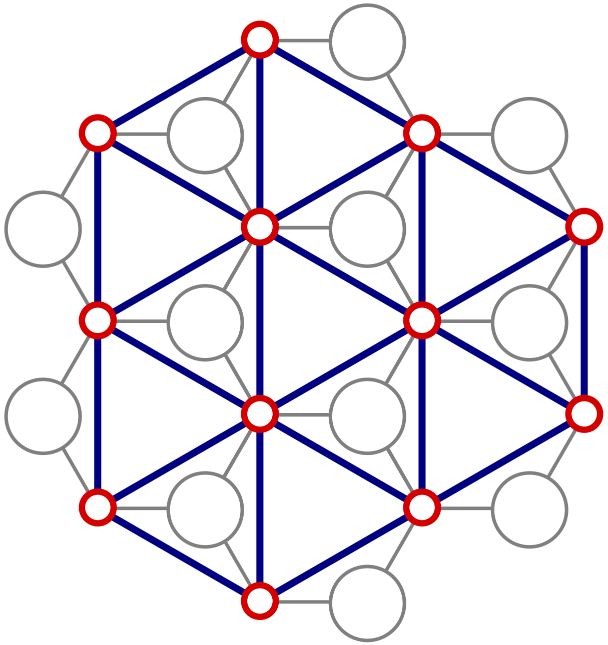
CO + AF

not yet checked for spin liquid states

discussion / outlook

effective lattices through charge ordering (off half filling)





VMC - spontaneous ordering

charge : insulating and conducting states, all fillings

dimer : only insulating states, half filling

magnetic : ?