分子結晶における電荷秩序の融解と超伝導に関する密度行列繰り込み群による研究

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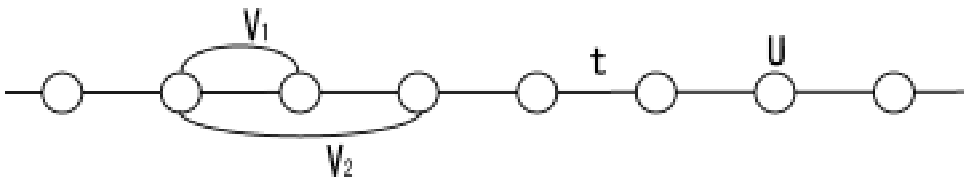
1. **Extended Hubbard model on a single chain (TMTTF)**
2. **Extended Hubbard model on a double chain (spin-gap liquid)**
3. **Extended Hubbard (*t*-*J*) model on the anisotropic triangular lattice (superconducting correlations)**
4. **Future directions**

Melting of CO due to charge frustration, leading to anomalous metallic states.
DMRG method

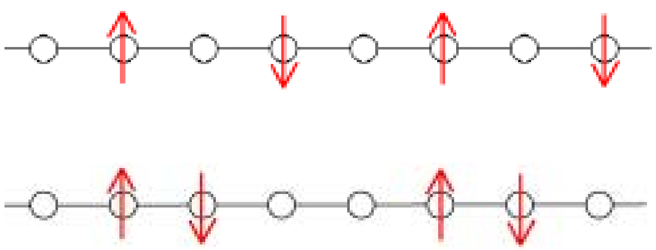
Extended Hubbard model on a single chain

Melting of CO due to charge frustration
Precise determination of the ground-state phase diagram and K_ρ



1/4 filling

CO patterns at quarter filling

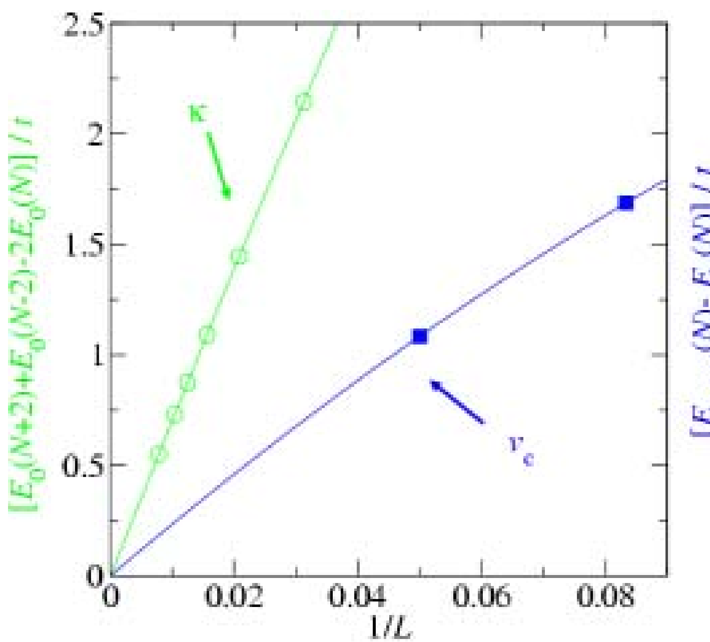


$4k_F$-CDW

$2k_F$-CDW

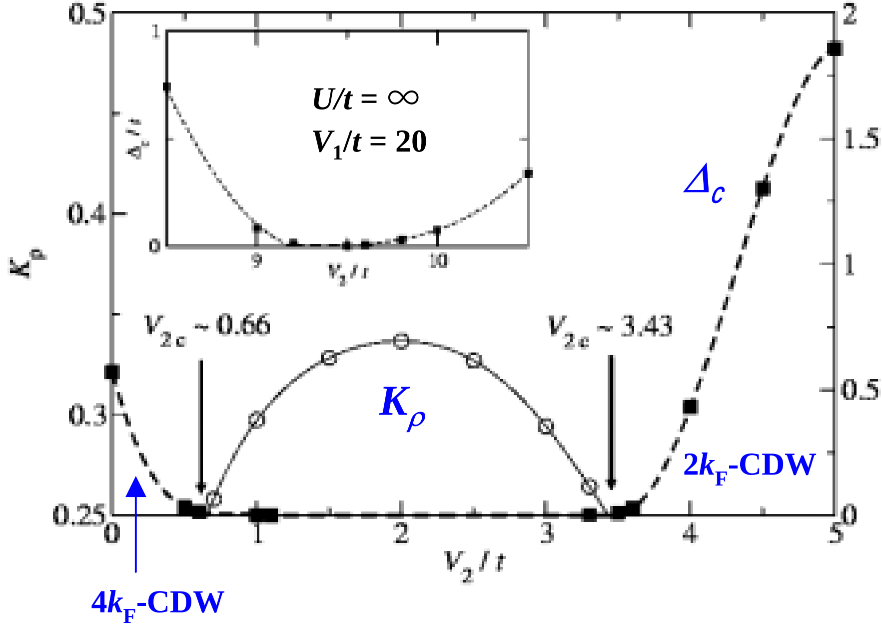
K_ρ is determined from compressibility κ (DMRG) and charge velocity v_c (ED).

DMRG method: up to 128 sites, m=500, $\delta E < 1.0 \times 10^{-4}\, t$

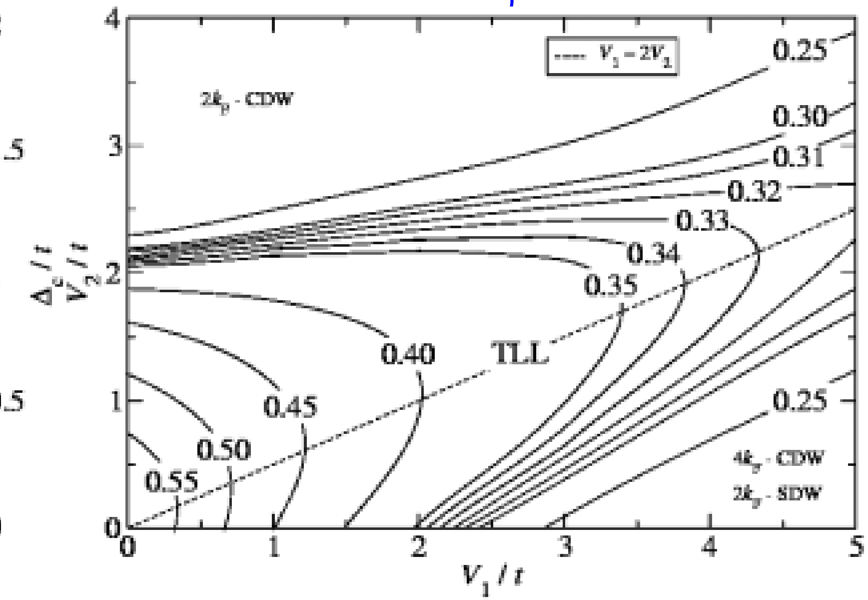


Ground-state phase diagram and K_ρ

***U*/*t*=10, *V*$_1$/*t*=4, (Inset: *U*/*t*=∞, *V*$_1$/*t*=20)**



Contour plot of K_ρ ***U*/*t*=10**



TLL always with K_ρ > 0.25.
Charge gap opens and CDW occurs at K_ρ=0.25.

Experiment:

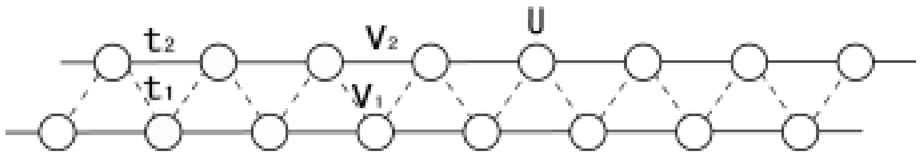
TMTSF: K_ρ = 0.23 (Schwartz *et al*.: PRB 58, 1261 (1998))

TTF-TCNQ: K_ρ = 0.17 (Sing *et al*.: PRB 68, 125111 (2003))

***U*-independent. Filling dependence?**

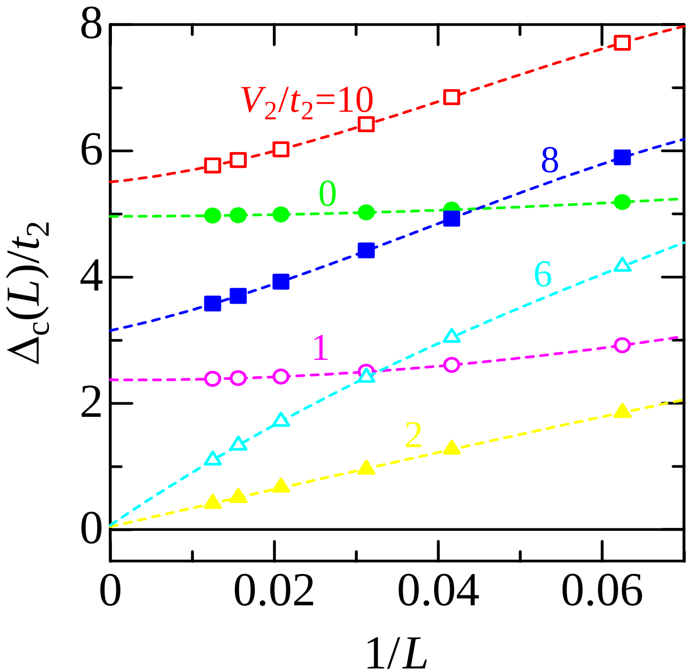
Double-chain Hubbard model

S. Nishimoto and Y.O.: PRB 68 (2003) 235114.

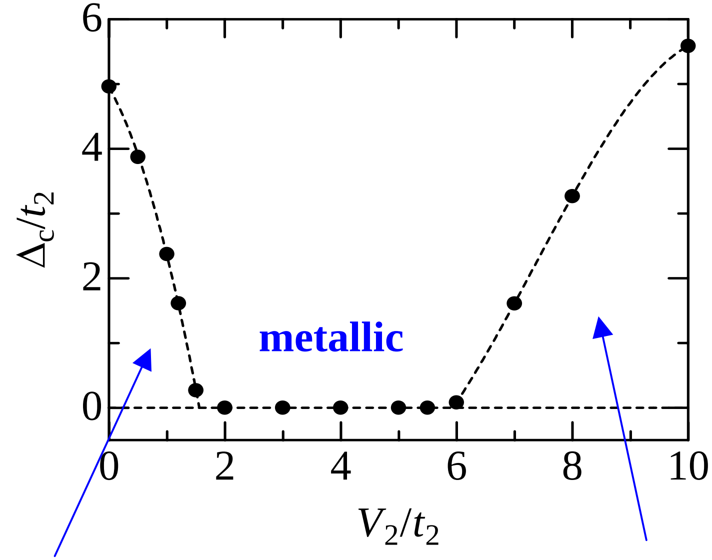


CuO double chains of nonsuperconducting $PrBa_2Cu_4O_8$

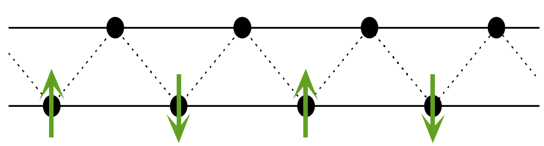
$t_2 >> t_1$, U/t_2=20, V_1/t_2=5, quarter filling



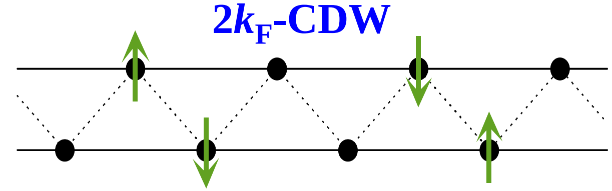
$$\Delta_c = \lim_{L\to\infty} \Delta_c(L)$$



$4k_F$-CDW



$2k_F$-CDW

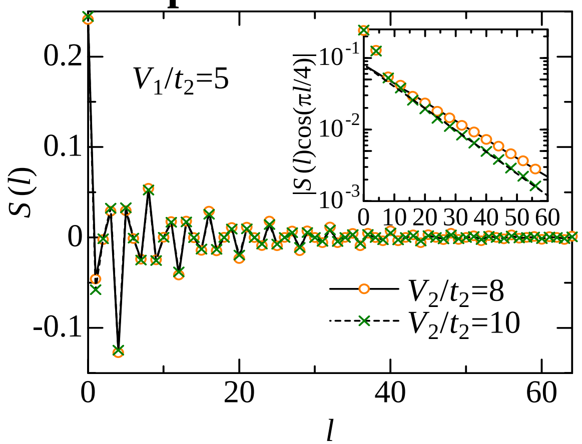


Ground-state phase diagram

S. Nishimoto and Y.O.: PRB 68 (2003) 235114

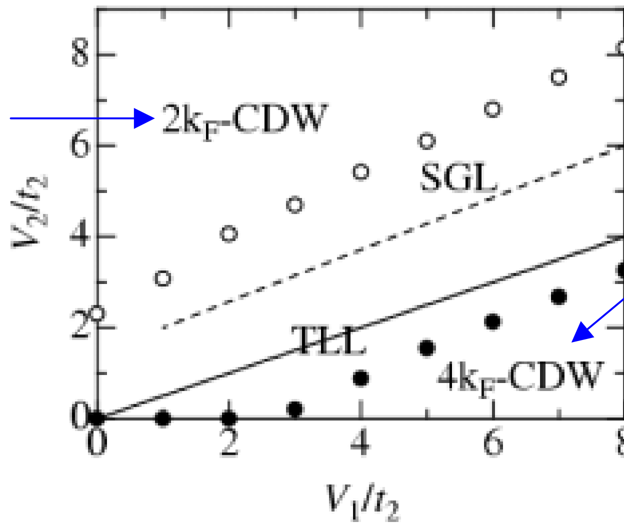
Presence of spin-gap liquid phase

Spin correlation

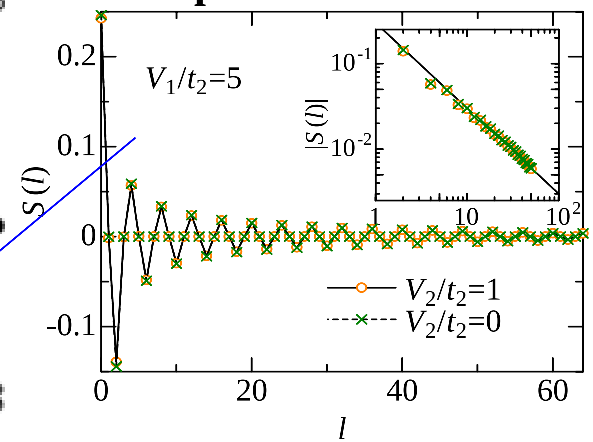


Exponential decay

⇒ Heisenberg ladder



Spin correlation

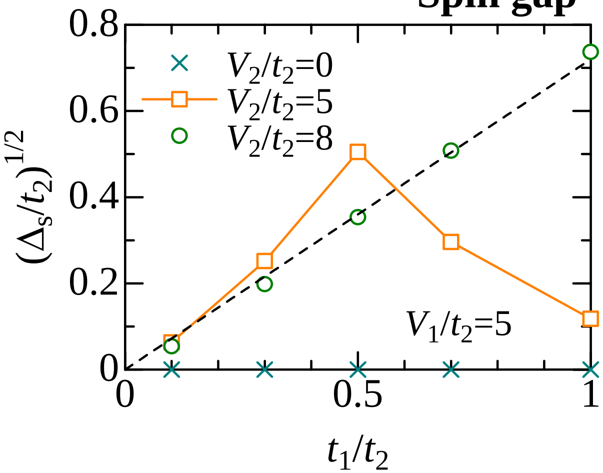


Power-low decay

⇒ Heisenberg chain

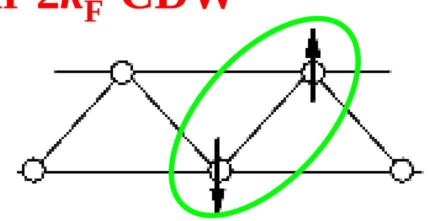
$$\Delta_s = \lim_{L\to\infty} \Delta_s(L)$$

Spin gap



$\Delta_s \propto t_1^2$

near 2k_F-CDW

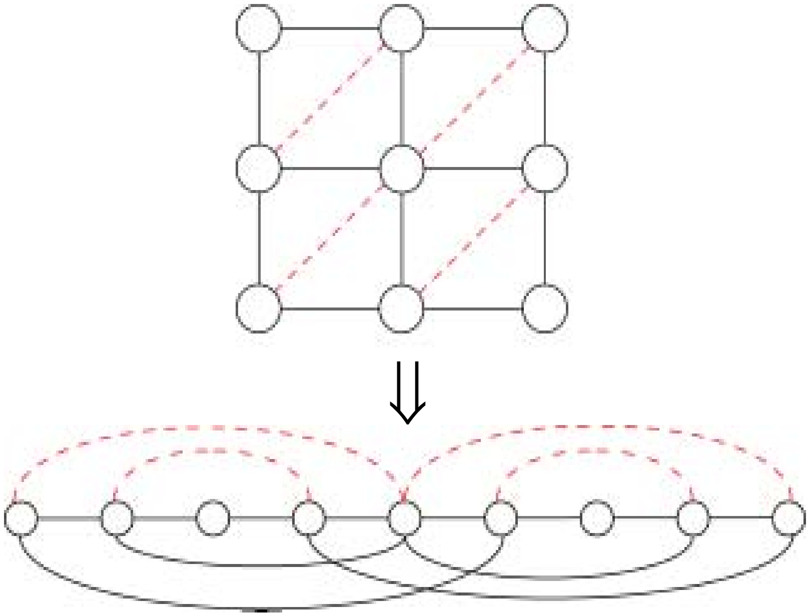


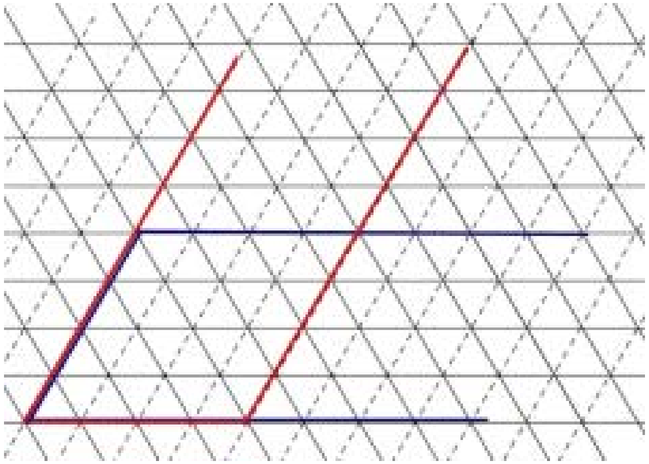
Mobile singlet pairs

Anisotropic triangular lattices

Is DMRG applicable to 2D models?

Mapping to the 1D system with
long-range interactions



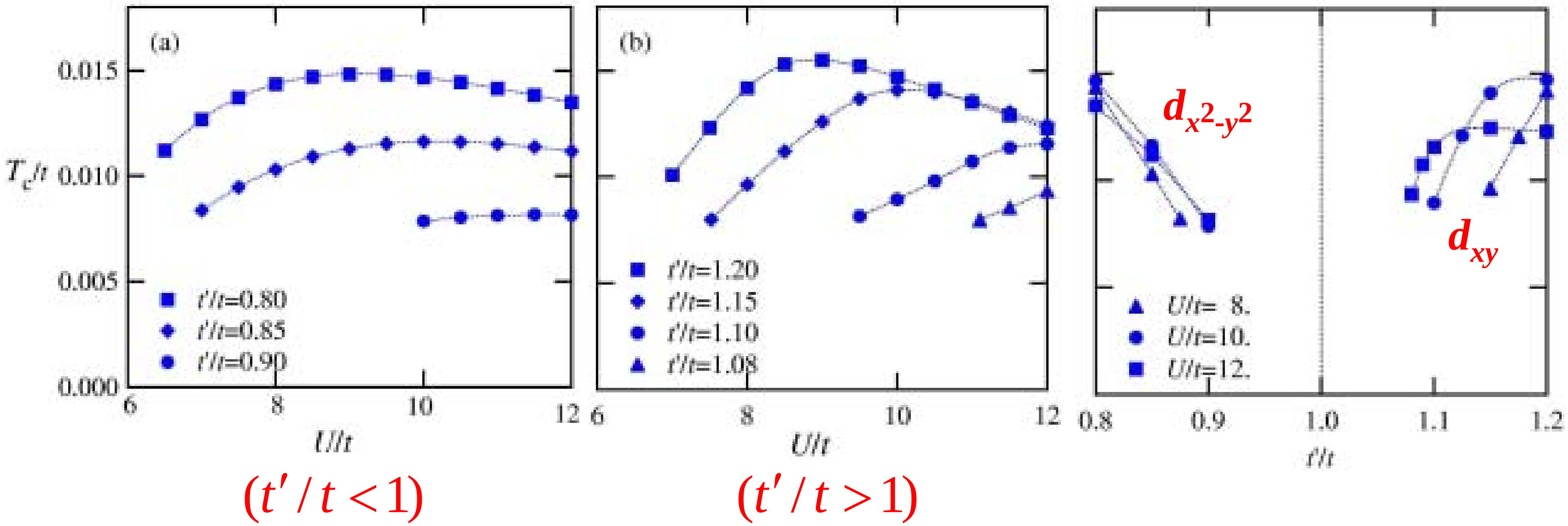


e.g.: 24×4 cluster, *m*=1600

We can use the standard DMRG method in 1D.

FLEX approximation for the *t-t'-U* Hubbard model at half filling

H. Kondo and T. Moriya: JPSJ 73 (2004) 812



$\Rightarrow$ **Symmetry of order parameters changes**

from $t'/t < 1$ to $t'/t > 1$; $d_{x^2-y^2} \Rightarrow d_{xy}$

SC order parameters

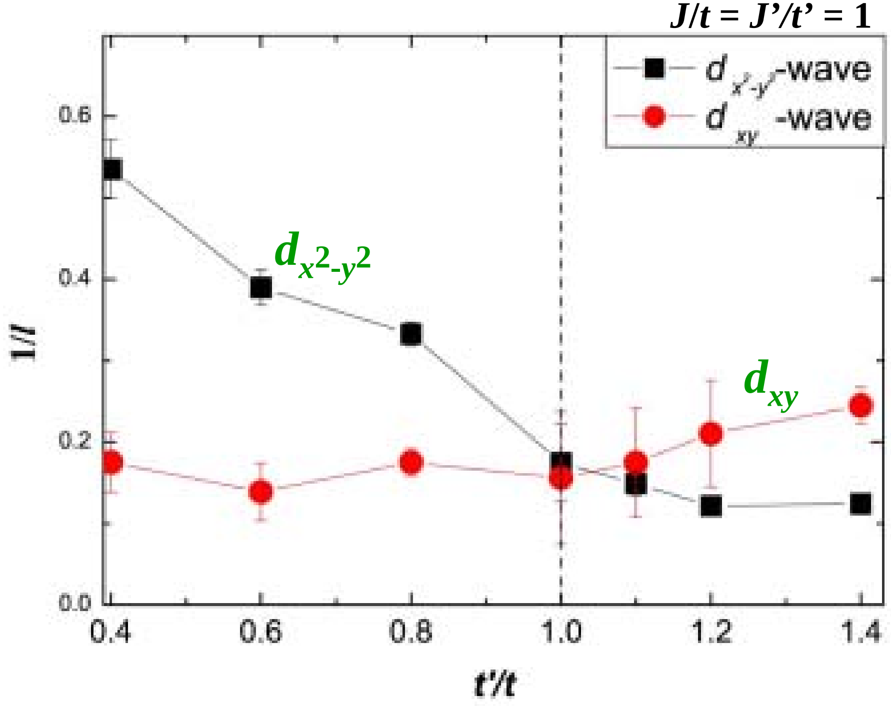
Anisotropic triangular-lattice
***t-J* model at *n* = 0.83.**

We assume

$$\left\langle \Psi \middle| \Delta_i^{x^2-y^2} (\Delta_{i+r}^{x^2-y^2})^\dagger \middle| \Psi \right\rangle \propto r^{-l}$$

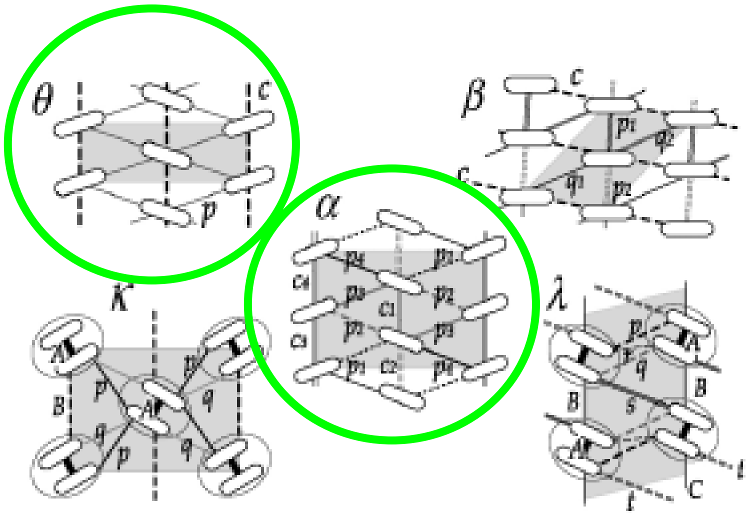
$$\left\langle \Psi \middle| \Delta_i^{xy} (\Delta_{i+r}^{xy})^\dagger \middle| \Psi \right\rangle \propto r^{-l}$$

and evaluate the value of $1/l$.



Symmetry of the SC correlations changes from d_{x2-y2} to d_{xy} as we go from $t'/t<1$ to $t'/t>1$.

Future directions



Extended Hubbard model at ¼ filing on **the anisotropic triangular lattices** **by** **DMRG method**

θ-type (BEDT-TTF)$_2$X
α-type, etc.

⇒ **CO melting**
⇒ **Charge fluctuations**
⇒ **Mechanism of superconductivity**

C. Hotta: JPSJ: 72 (2003) 840.