Metal-insulator transition and Fermi surface evolution in frustrated triangular-based lattices

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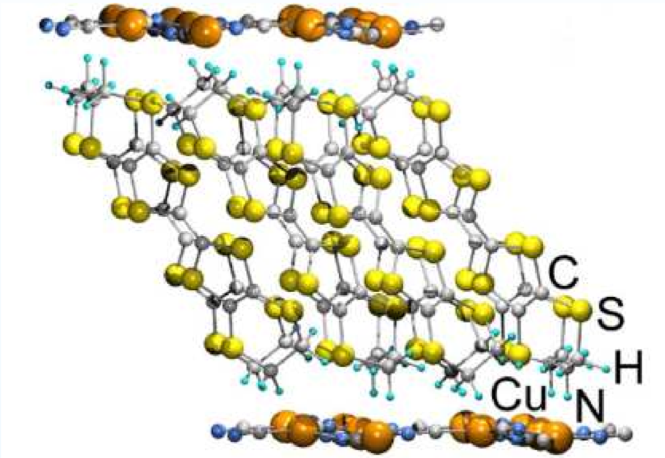
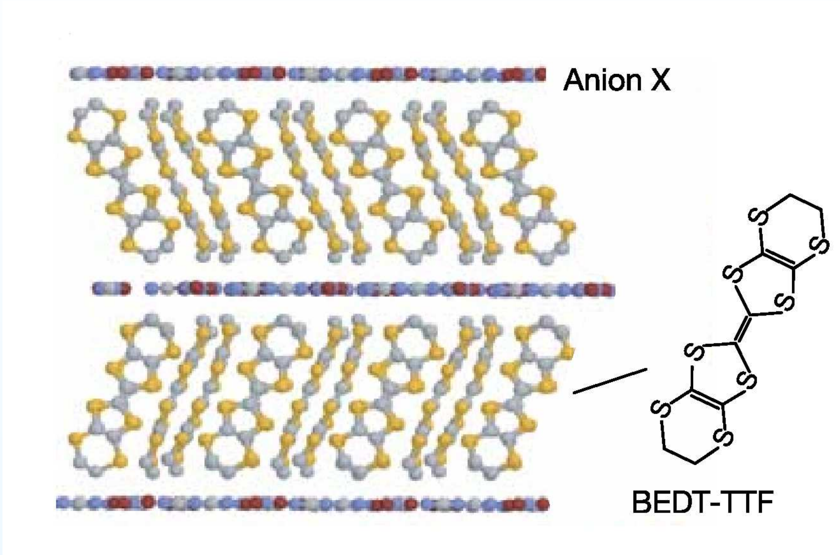
Outline

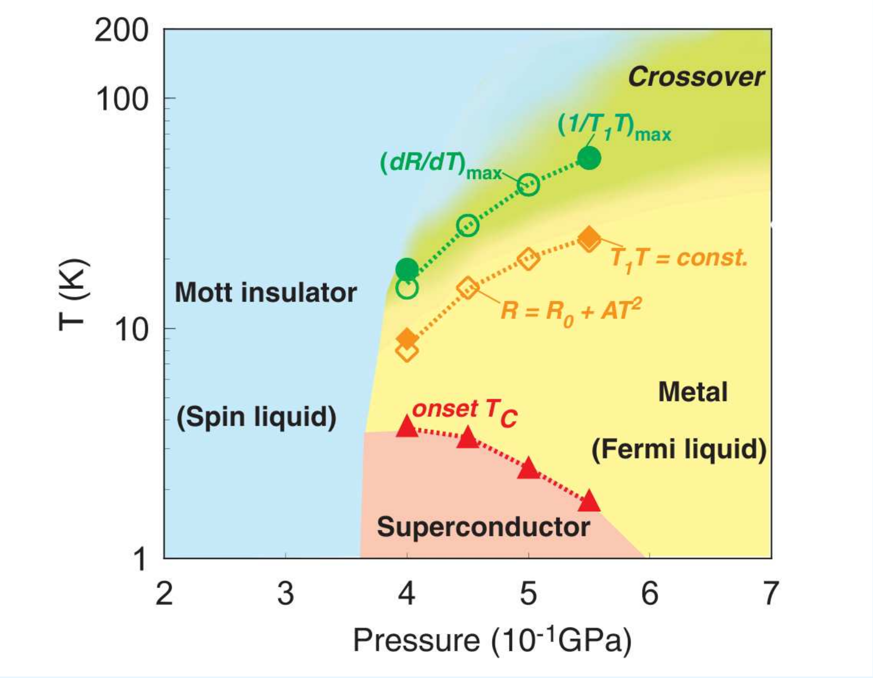




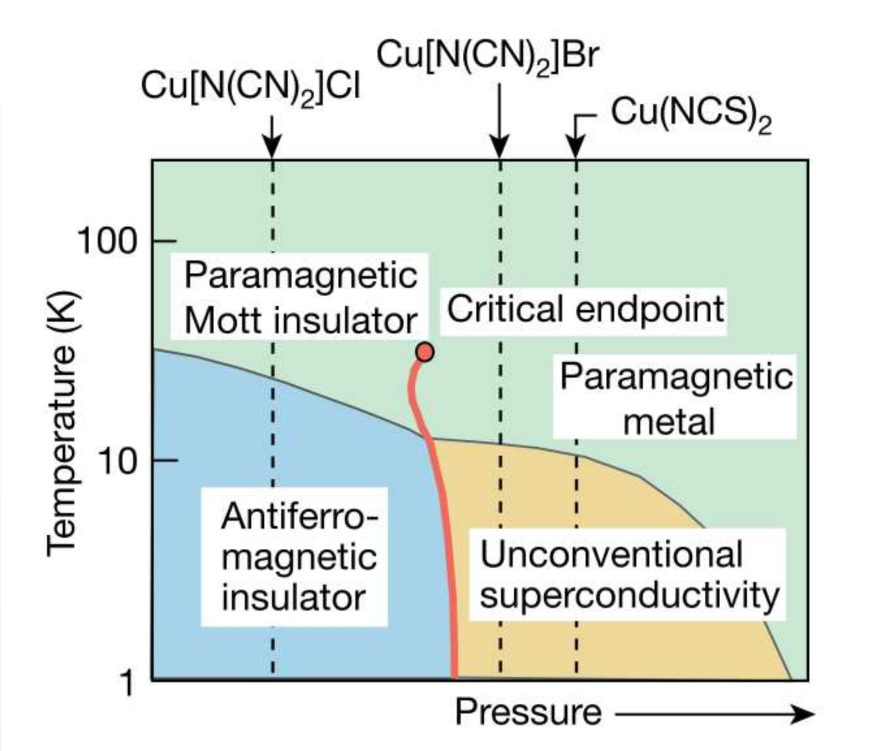
- The $\kappa-$(ET)$_2$X family
- The Hubbard model on the triangular lattice
- Ground-state wave functions in Variational Monte Carlo
- Phase diagram for the anisotropic triangular lattice
- Magnetic properties in the insulating phase
- Fermi surface reconstruction at the MIT

The $\kappa-$(ET)$_2$X family: phase diagrams

$\kappa-$(ET)$_2$Cu$_2$(CN)$_3$



Y. Kurosaki *et al.*, PRL 95, 177001 (2005)



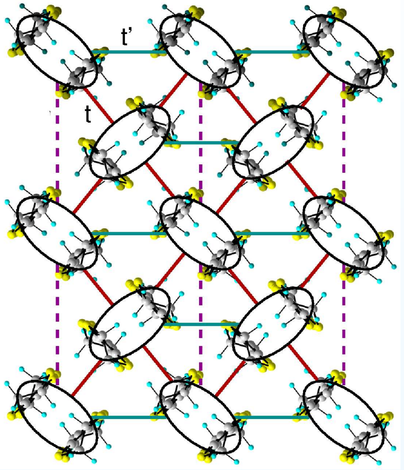
F. Kagawa *et al.*, Nature 436, 534 (2005)

$\kappa-$(ET)$_2$Cu$_2$(CN)$_3$ is an insulator without magnetic order at ambient pressure, down to $T \simeq 32mK$ ($T \ll \Theta_{CW} \simeq 250K$)

Y. Shimizu *et al.*, PRL 91, 107001 (2003)

The $\kappa-$(ET)$_2$X family: model structure

- 2D layers of ET molecules with a strong dimerization
- The dimers form a triangular lattice with one hole per dimer and hopping integrals t and t' (single-band model)



Estimates of the hopping integrals t and t' in DFT

H.C. Kandpal *et al.*, PRL 103, 067004 (2009); K. Nakamura *et al.*, JPSJ 78, 083710 (2009)

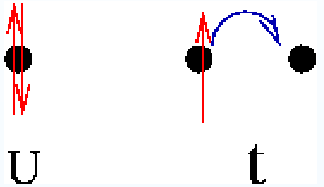
- $t'/t \simeq 0.83$ for X=$Cu_2(CN)_3$
- $t'/t \simeq 0.58$ for X=$Cu(SCN)_2$
- $t'/t \simeq 0.44$ for X=$Cu[N(CN)_2]Cl$

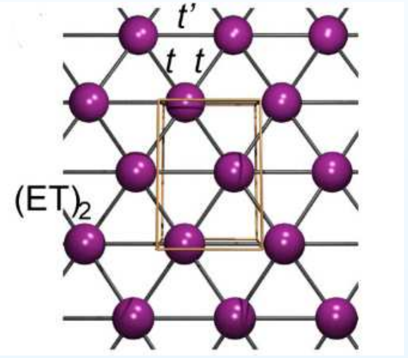
Estimates of the on-site Coulomb repulsion U are controversial

- $U/t \simeq$ 12–15 in JPSJ 78, 083710 (2009)
- $U/t \simeq$ 5–7 in PRL 103, 067004 (2009)

The single-band Hubbard model

$$\mathcal{H} = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$





- $t'/t = 0.85$ and $t'/t = 0.6$
  relevant for $\kappa-$(ET)$_2$Cu$_2$(CN)$_3$ and $\kappa-$(ET)$_2$Cu(SCN)$_2$
- One particle per lattice site

Numerical technique to determine the ground-state properties:
Variational Monte Carlo

J. Liu, J. Schmalian, and N. Trivedi, PRL 94, 127003 (2005)

The variational wave functions

$$|\Psi\rangle = \mathcal{J}\mathcal{J}_s|\mathcal{MF}\rangle$$

M. Capello *et al.* PRL 94, 026406 (2005)

$|\mathcal{MF}\rangle$ is the ground state of a mean-field Hamiltonian

$$(1)\quad \mathcal{H}_{BCS} = \sum_{i,j,\sigma} \tilde{t}_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} + \sum_{i,j} \Delta_{ij} c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} + h.c.$$

$$(2)\quad \mathcal{H}_{AF} = \sum_{i,j,\sigma} \tilde{t}_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. + \Delta_{AF} \sum_i \mathbf{n}_i \mathbf{S}_i$$

$$\mathcal{J}_s = \exp\left[-\frac{1}{2}\sum_{i,j} u_{i,j} S^z_i S^z_j\right] \qquad \mathcal{J} = \exp\left[-\frac{1}{2}\sum_{i,j} v_{ij} n_i n_j\right]$$

+ Backflow correlations in the Slater determinant

Redefinition of the electronic coordinates

R.P. Feynman and M. Cohen, Phys. Rev. 102, 1189 (1956)

Metal or insulator?

Ansatz for the low-energy excitations

$$|\Psi_q\rangle = n_q|\Psi_0\rangle$$

Feynman, Phys. Rev. (1954)

f-sum rule

$$\Delta_q = \frac{\langle\Psi_q|(H-E_0)|\Psi_q\rangle}{\langle\Psi_q|\Psi_q\rangle} = \frac{\langle\Psi_0|[n_{-q},[H,n_q]]|\Psi_0\rangle}{2N_q} \sim \frac{q^2}{N_q}$$

$$N_q = \frac{\langle\Psi_0|n_{-q}n_q|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

$N_q \sim |q| \Rightarrow \Delta_q \to 0 \quad \Rightarrow$ metal

$N_q \sim q^2 \Rightarrow \Delta_q$ is finite $\Rightarrow$ insulator (upper bound)

Difference in the electron organization

Reatto-Chester relation for N_q and Jastrow factor

$$N_q = \frac{\langle \Psi | n_{-q} n_q | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

RPA Reatto and Chester, Phys. Rev. (1967)

- **For continuous systems**
- **In the weak-coupling regime**

$$N_q = \frac{N_q^0}{1 + 2v_q N_q^0} \sim \frac{1}{v_q}$$

$N_q^0 = \frac{\langle \mathcal{D} | n_{-q} n_q | \mathcal{D} \rangle}{\langle \mathcal{D} | \mathcal{D} \rangle} \sim |q|$ **is the uncorrelated structure factor**

$v_q \sim 1/q^2$ cannot be found with RPA for short-range models

On the continuum

for free electrons

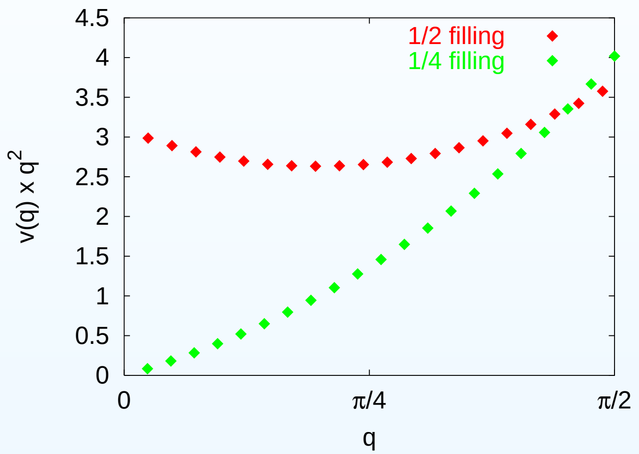
Gaskell,

Proc. Phys. Soc. (1961)

$$2v_q = -\frac{1}{N_q^0} + \sqrt{\frac{1}{(N_q^0)^2} + \frac{4m\Omega_q}{(\hbar q)^2}} \sim \frac{1}{|q|}$$

Optimized Jastrow parameters

Hellberg and Mele (1991); Yokoyama and Ogata (1991); Gros and Valenti (1993)



1D for $U/t = 10$

At finite doping $v_q \sim 1/|q|$

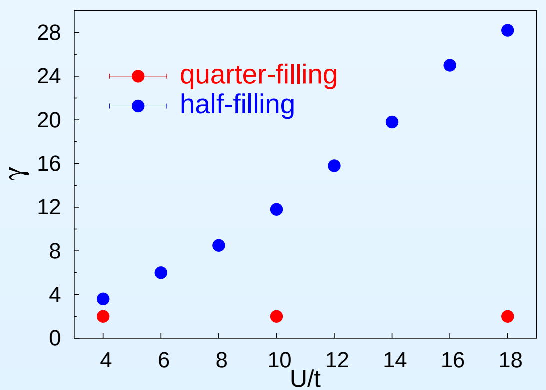
At half filling $v_q \sim 1/q^2$

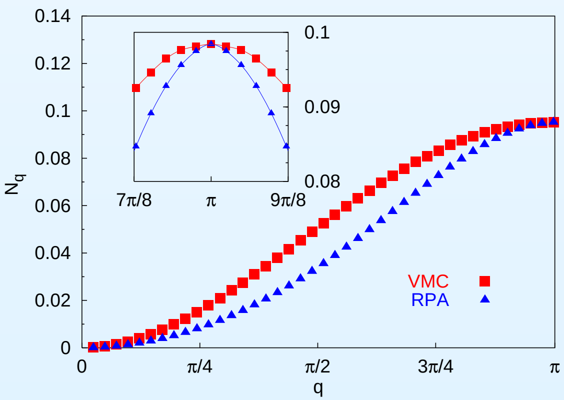
OK for the metal (finite doping)

Wrong for the insulator!

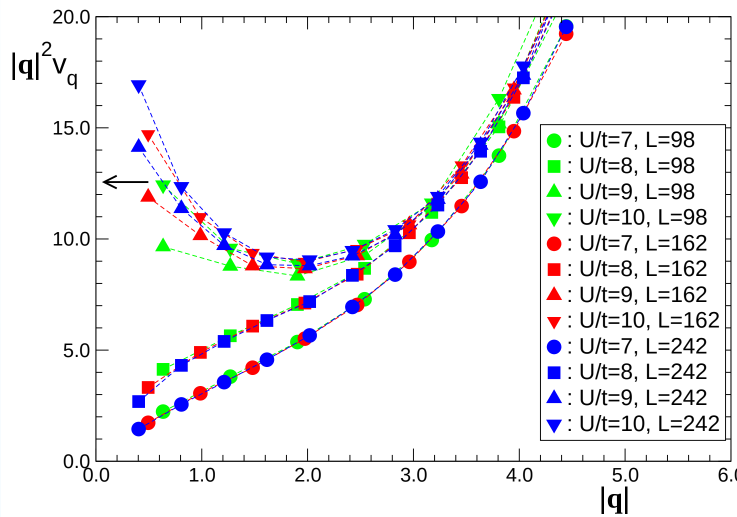
QUALITATIVELY valid for small q

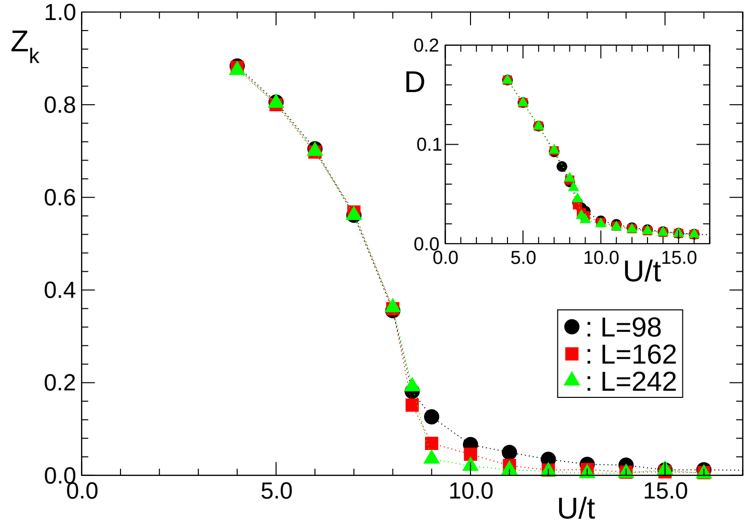
$$N_q = \frac{N_q^0}{1 + \gamma v_q N_q^0}$$





Two-dimensional (paramagnetic) Hubbard model





$$Z_k = \frac{|\langle \Psi_{N-1} | c_{k,\sigma} | \Psi_N \rangle|^2}{\langle \Psi_N | \Psi_N \rangle \langle \Psi_{N-1} | \Psi_{N-1} \rangle} \quad \textit{with} \quad |\Psi_{N-1}\rangle = \mathcal{J}\, c_{k,\sigma}\, |\mathcal{FS}\rangle$$

- $U/t \lesssim 8.5$: $v_q \sim \frac{1}{|q|}$ with Z_k finite: **FERMI LIQUID**
- $U/t \gtrsim 8.5$: $v_q \sim \frac{1}{q^2}$ with vanishing Z_k: **MOTT INSULATOR**

Backflow correlations in variational wave functions

Correlation between empty sites and doubly occupied sites
inside the mean-field variational wave function $|BCS\rangle$ or $|AF\rangle$

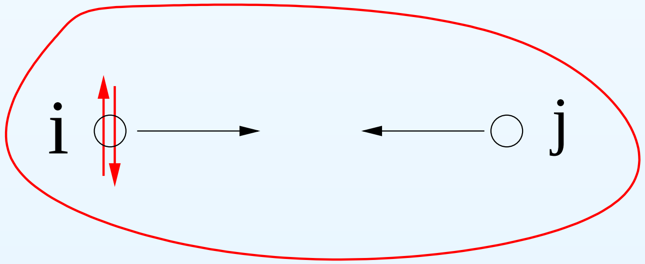
Redefinition of the electronic coordinates $\mathbf{r}$

R.P. Feynman and M. Cohen, Phys. Rev. 102, 1189 (1956)

$$\boldsymbol{r}^b_{i,\sigma} = \epsilon \boldsymbol{r}_{i,\sigma} + \eta \sum_j t_{ij} D_i H_j (\boldsymbol{r}_{j,\sigma} - \boldsymbol{r}_{i,\sigma})$$

$$D_i = n_{i,\uparrow} n_{i,\downarrow}$$

$$H_j = (1 - n_{j,\uparrow})(1 - n_{j,\downarrow})$$



On the lattice, electronic positions are limited to lattice sites!!

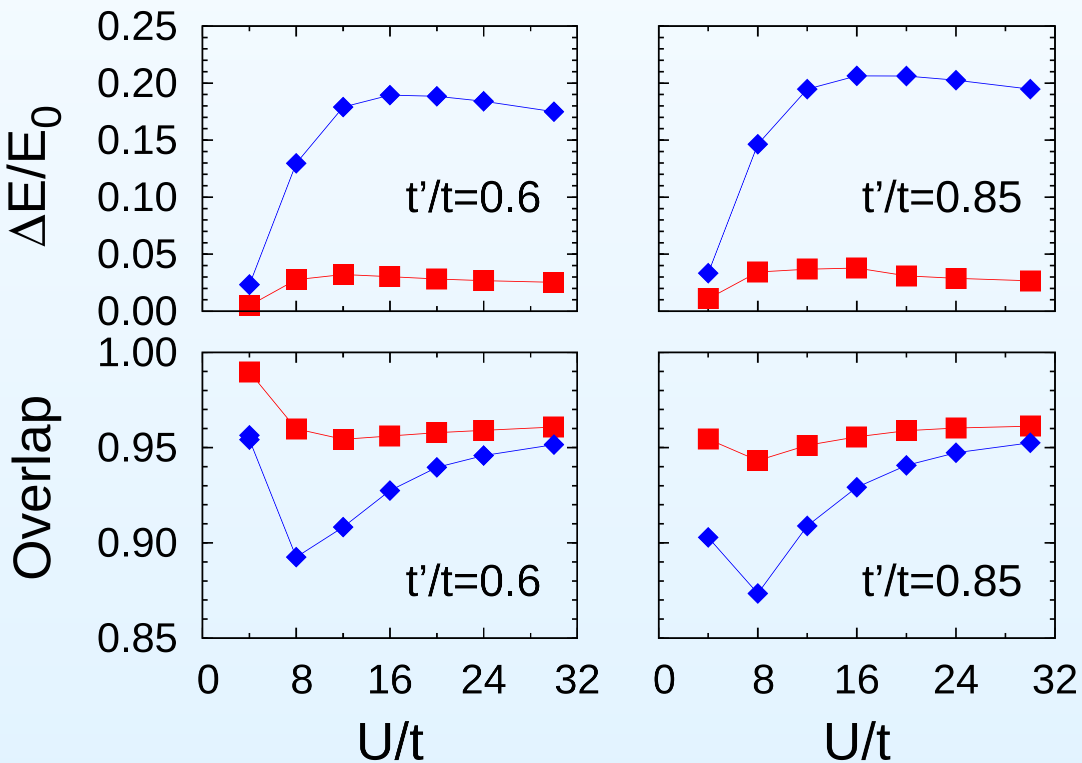
$$\phi_k(\boldsymbol{r}^b_\alpha) \simeq \phi^b_k(\boldsymbol{r}_\alpha) \equiv \phi_k(\boldsymbol{r}_\alpha) + \sum_\beta c_{\alpha,\beta} \phi_k(\boldsymbol{r}_\beta)$$

L.F. Tocchio *et al.*, PRB 78, 041101(R) (2008)

Variational results vs exact ones

(Lanczos on an 18-site lattice)

Backflow correlations strongly improve $|\Psi_{BCS}\rangle$
(a further improvement may be obtained by GFMC)

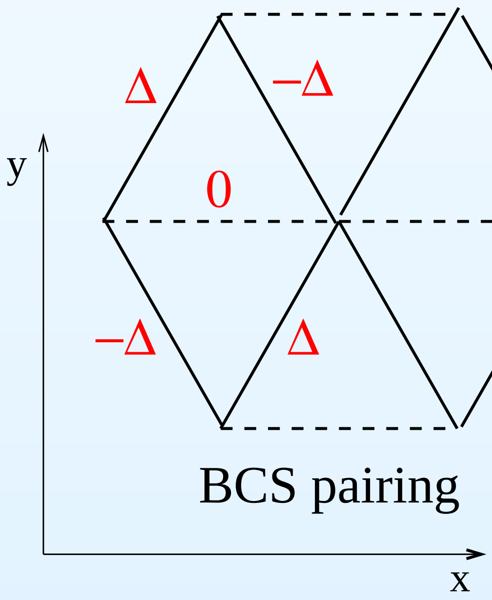


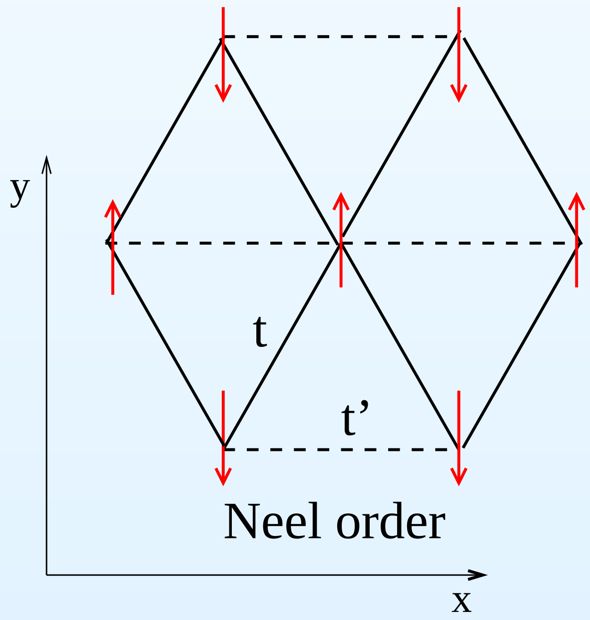
$\Delta E = E_{\text{var}} - E_0$; blue triangles=no backflow red circles=backflow

BCS pairing and magnetic order

The unfrustrated character is stable from $t' = 0$ to $t'/t \simeq 0.9$:

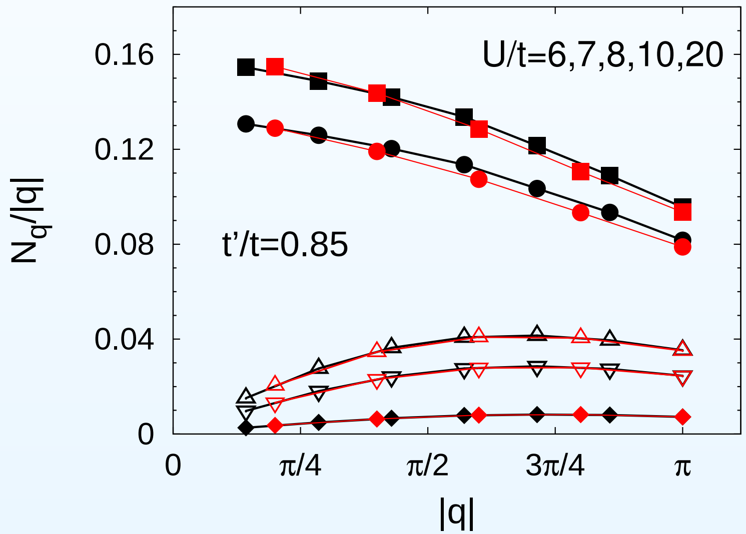
- The BCS pairing has $d_{x^2-y^2}$ symmetry
- The best magnetic order is collinear (Néel order)

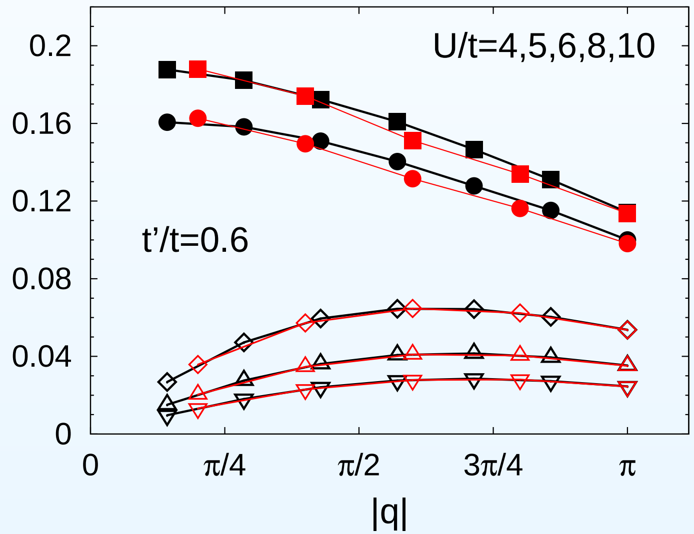




Metal-insulator transition

$$N(q) = \langle n_q n_{-q} \rangle \quad n_q = \frac{1}{\sqrt{N}} \sum_r e^{iqr} n_r$$





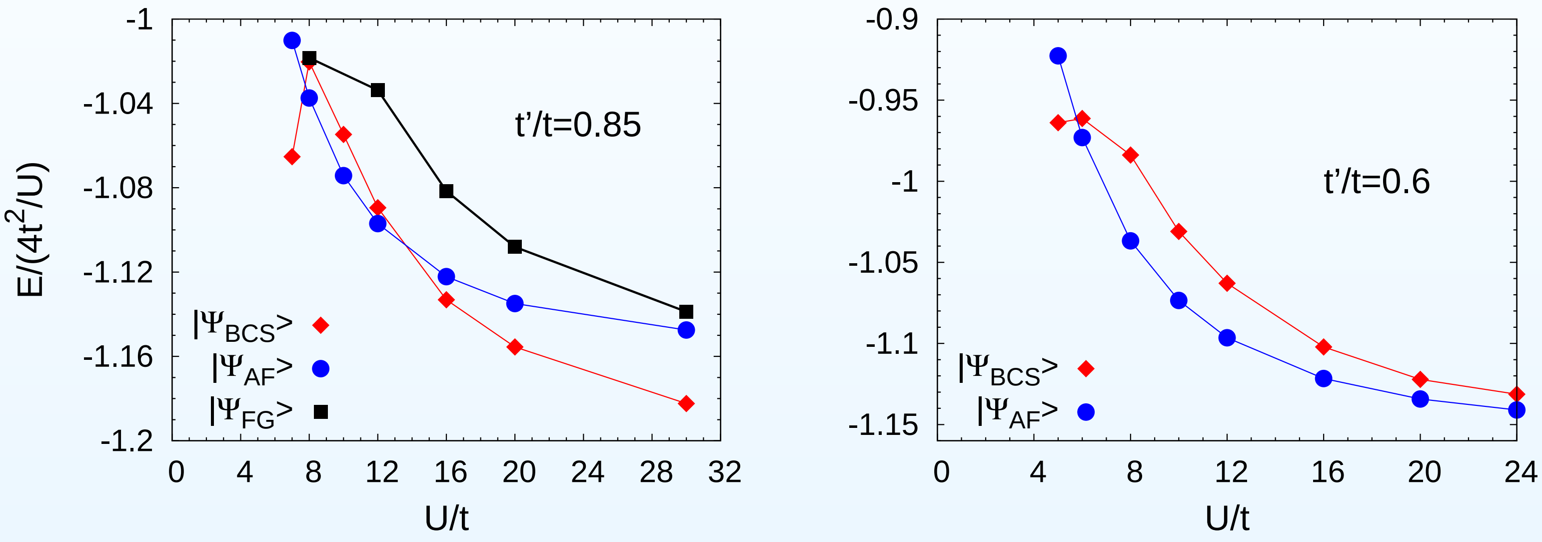
- $E_q - E_0 \simeq \frac{q^2}{N(q)}$
- $N(q) = \langle n_q n_{-q} \rangle \sim q^2$ for $|q| \to 0$ in the insulating (gapped) phase
- $N(q) = \langle n_q n_{-q} \rangle \sim |q|$ for $|q| \to 0$ in the metallic (gapless) phase

Small BCS pairing in the metallic phase

The metallic phase is likely to be not superconducting

Variational phase diagram for $t'/t = 0.6$ and 0.85

Comparison between the variational energies



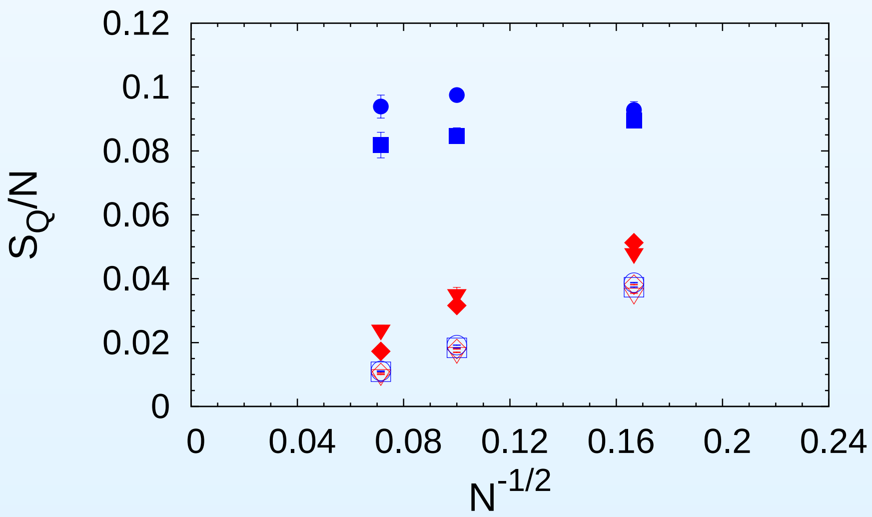
- $t'/t = 0.6$: $|\Psi_{AF}\rangle$ has always the best variational energy in the insulating phase
- $t'/t = 0.85$: Magnetic state for $7.5 \lesssim U \lesssim 13$; Spin-liquid state for $U \gtrsim 13$
- $t'/t = 0.85$: The BCS pairing is relevant in the insulating phase
- $t'/t = 0.85$: The spin-liquid state is favored only thanks to backflow correlations

Magnetic properties of the insulating phase

$$S(q) = \langle S^z_q S^z_{-q} \rangle \quad S^z_q = \frac{1}{\sqrt{N}} \sum_r e^{iqr} S^z_r$$

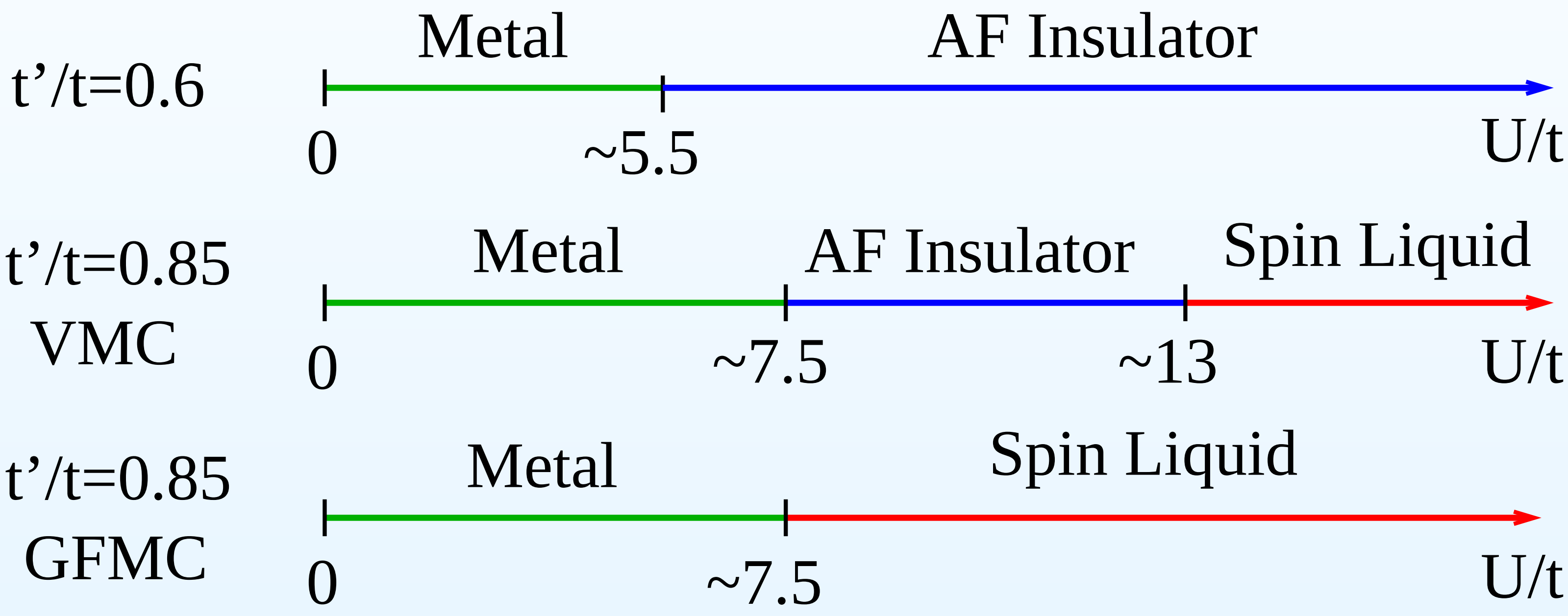
- VMC (empty symbols) with $|\Psi_{BCS}\rangle$ as a variational wave function
- Green's Function Monte Carlo (full symbols)

$S(q)$ has a peak at $Q = (\pi, \pi)$, corresponding to Néel order

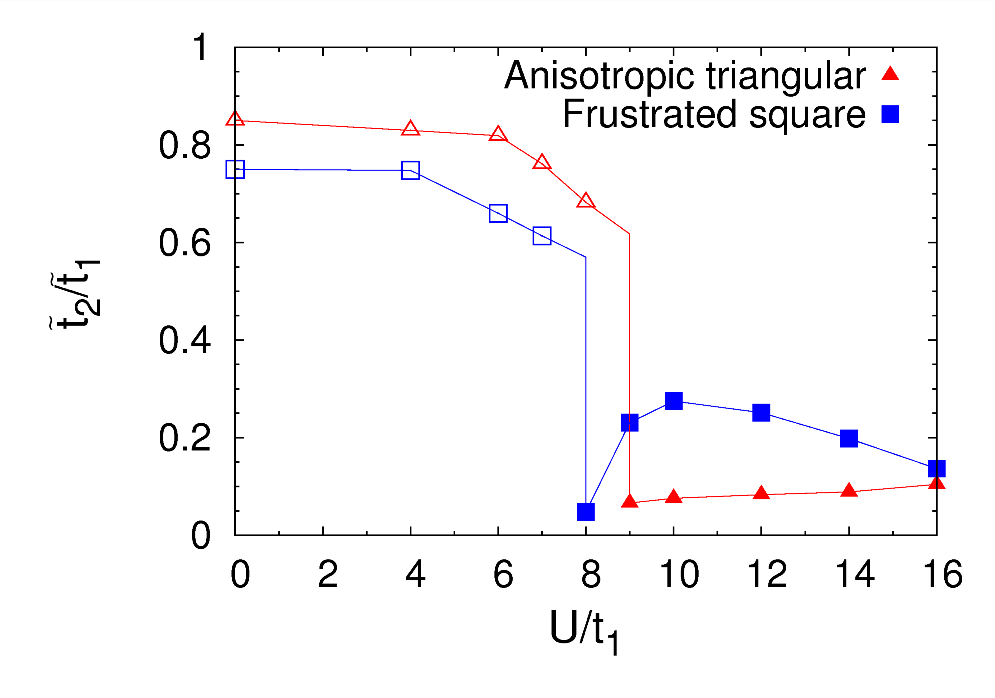


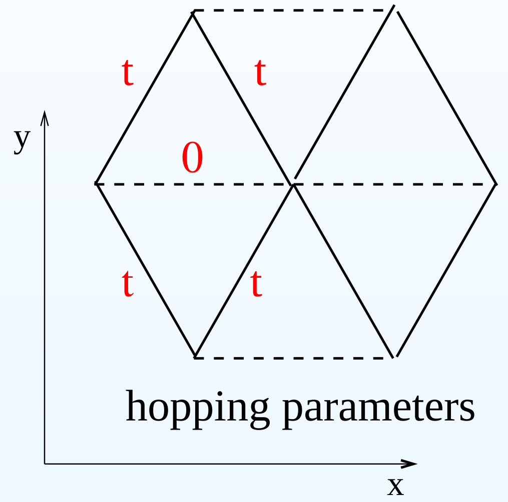
- No-long range magnetic order within VMC
- Finite magnetization at $t'/t = 0.6$ (blue symbols)
- No magnetic order at $t'/t = 0.85$ for $U/t = 10, 20$ (red symbols): the insulator is always non magnetic!

Phase diagram



Renormalization of the Fermi surface



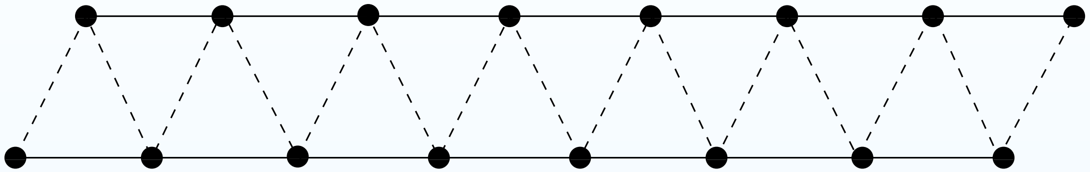


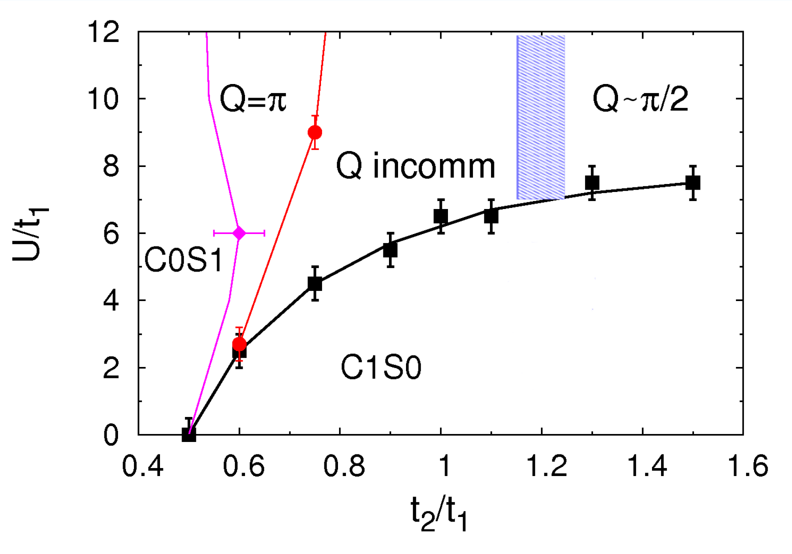
$$\mathcal{H}_{BCS} = \tilde{t}_1 \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. + \tilde{t}_2 \sum_{\langle\langle i,j \rangle\rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. + \ldots$$

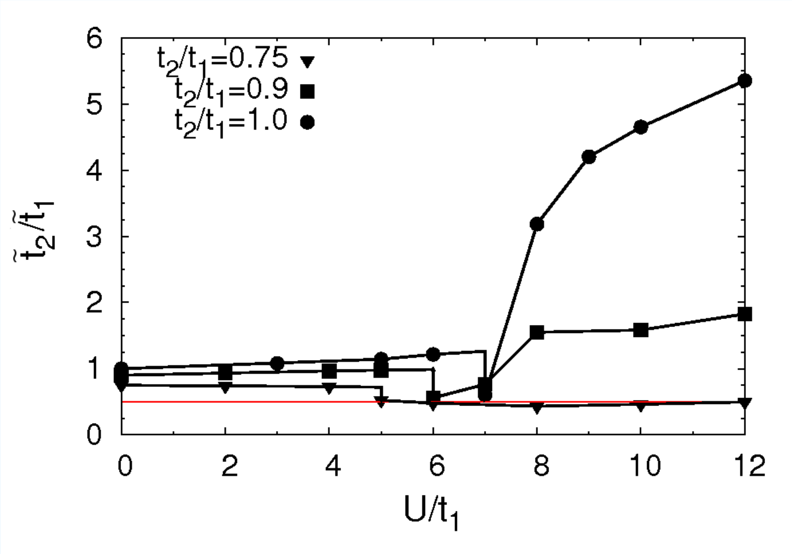
Perfect nesting of the underlying Fermi surface at the MIT

General for frustrated systems (also in the square lattice)

General result: the 1D zig-zag Hubbard model







In 1D $\tilde{t}_2/\tilde{t}_1 \to 1/2$ implies

perfect nesting of the Fermi surface at the MIT

Conclusions and outlook

- $t'/t = 0.85$: Spin-liquid insulating state
- $t'/t = 0.6$: Magnetic insulator with Néel order
- BCS pairing is relevant in the insulating phase
  (no spinon Fermi surface?)
- Spin liquid at strong couplings
- Isotropic triangular lattice?
  (spin liquid at intermediate couplings?)
  Misguich, Imada, Motrunich, Lee, Mila...
- Fermi surface nesting at the MIT (by doping?)