Numerical study of the phase diagram of extended Hubbard model on hexagonal lattice

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The model

Tight-binding Hamiltonian:

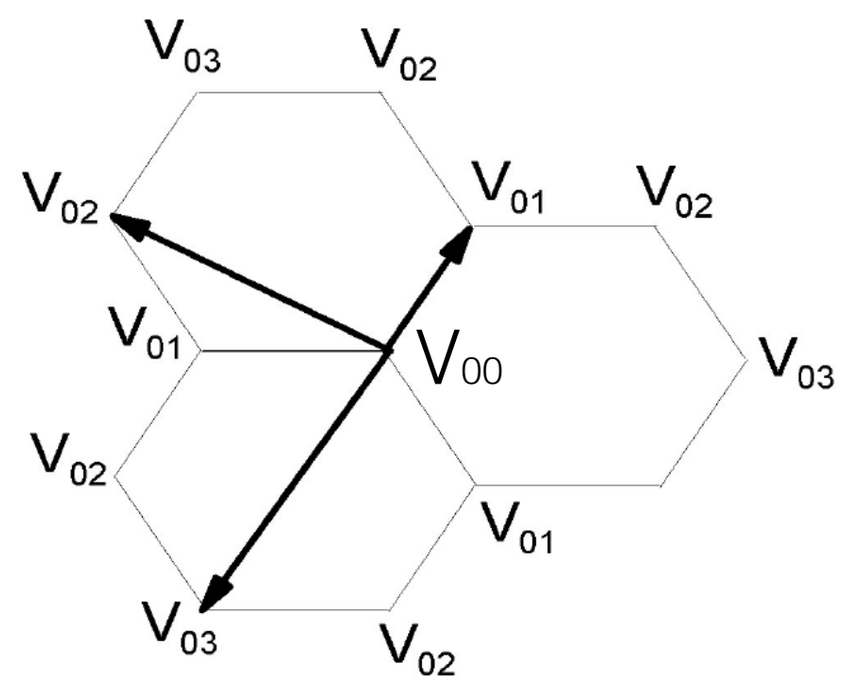
$$\hat{H}_{tb} = -\kappa \sum_{<x,y>,s} \left(\hat{a}^{+}_{y,s}\hat{a}_{x,s} + \hat{a}^{+}_{x,s}\hat{a}_{y,s}\right)$$

$a^{+}_{x,s}$ - creation operator for electrons with spin s

Interaction:

$$\hat{H}_C = \frac{1}{2}\sum_{x,y} V_{xy}\hat{q}_x\hat{q}_y$$

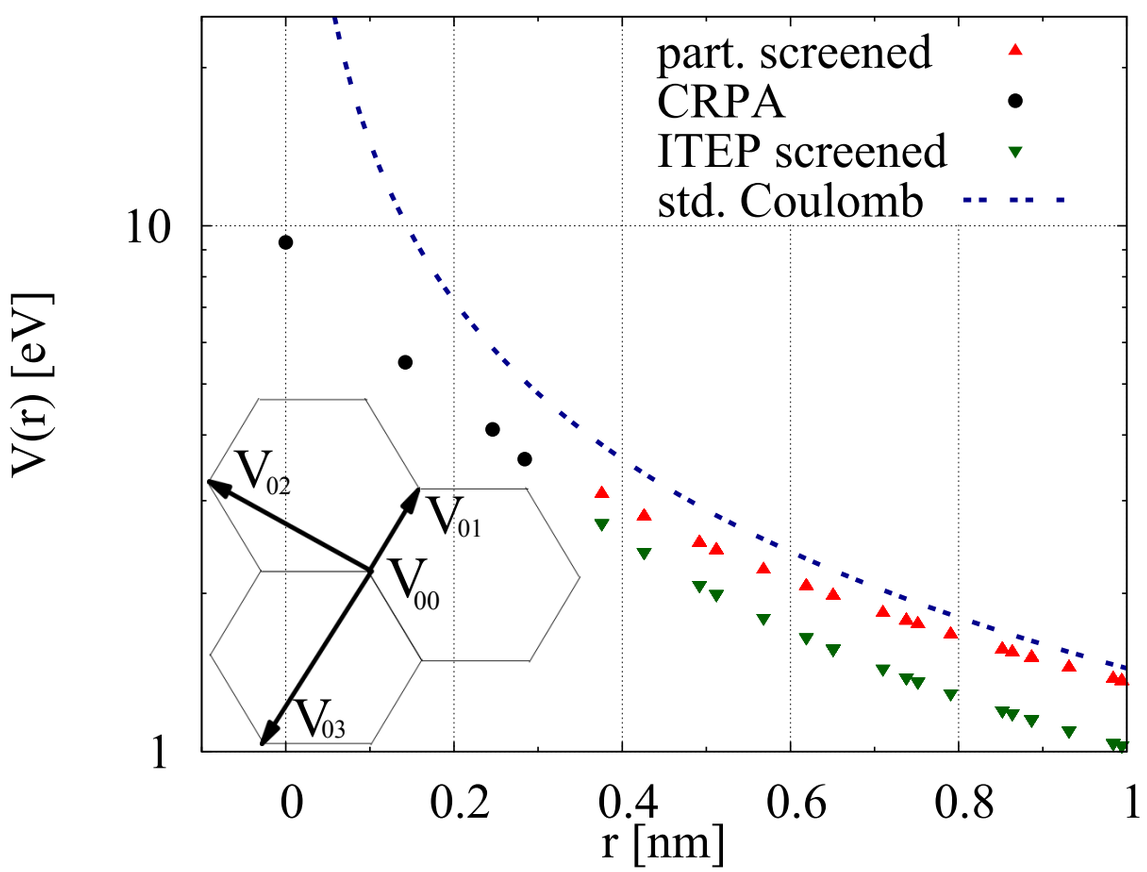
$$\hat{q}_x = \hat{a}^{+}_{x,1}\hat{a}_{x,1} + \hat{a}^{+}_{x,-1}\hat{a}_{x,-1} - 1$$

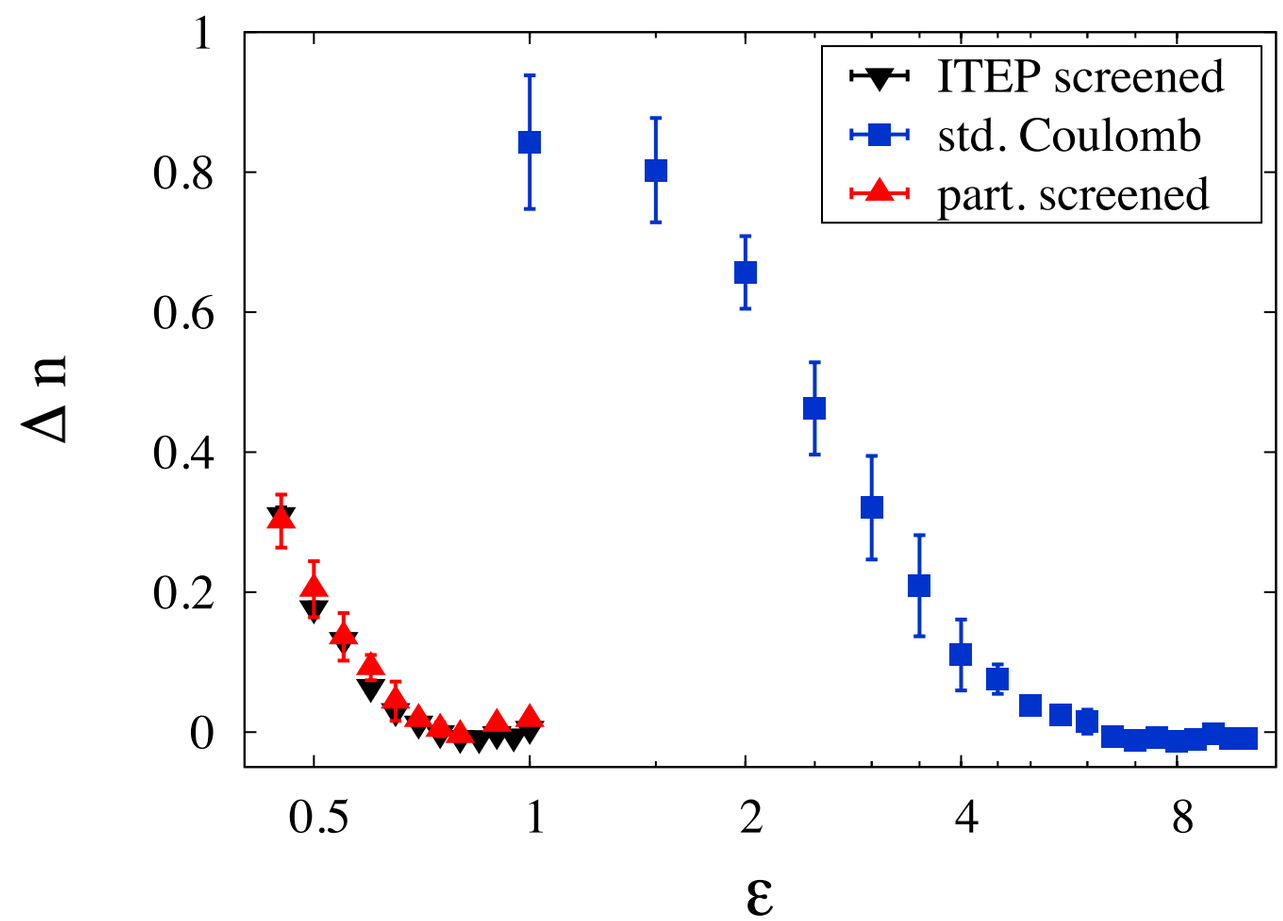


Only V_{00} and V_{01} are taken into account

Motivation (1)

Check the role of Coulomb interaction at various distances





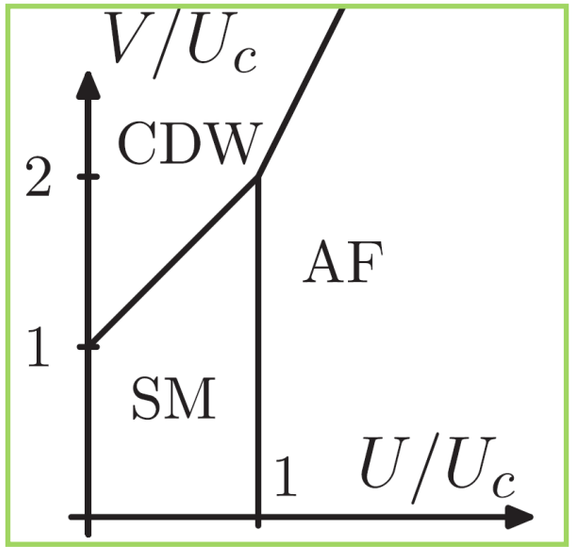
Ulybyshev et al, Phys. Rev. Lett. 111, 056801 (2013)
D. Smith and L. von Smekal, PRB 89, 195429 (2014)

Motivation (2)

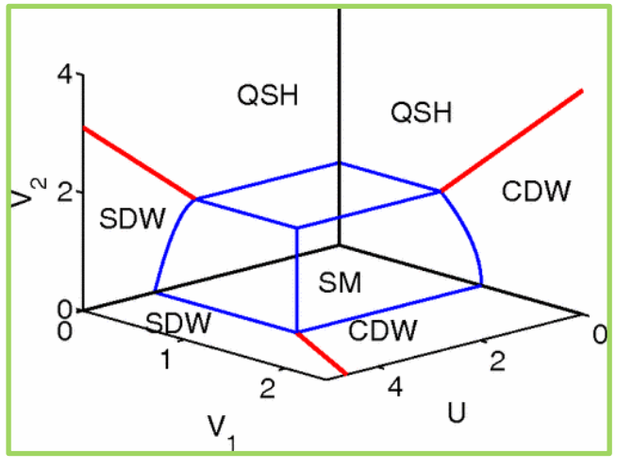
1) Minimally extended Hubbard model which still host AFM, SM and CDW phases.
2) Mapping of full long-range interaction into V_{00} potential: M. Schuler et. al., arXiv 1302.1437: effective on-site interaction = $V_{00} - V_{01}$

Previous calculations

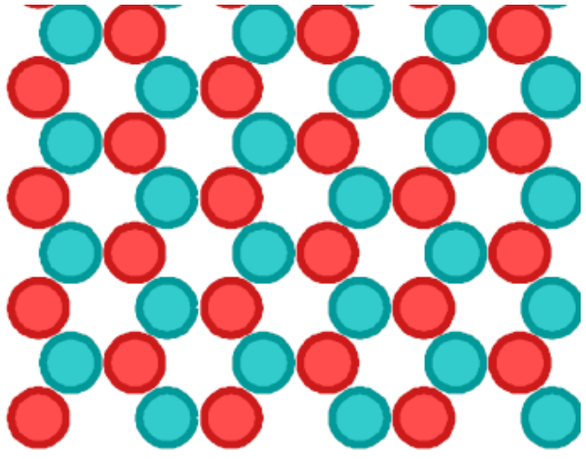
I. Herbut, arXiv: cond-mat/0606195: renormalization group study



Raghu et al, arXiv:0710.0030, appearance of topological phase



In low energy effective field theory:



$\bar{\psi}_a \sigma_3^{ab} \psi_b$ - antiferromagnetic condensate

$\bar{\psi}_a \psi_a$ - charge density wave

Quantum Monte Carlo basics

Discrete Euclidean time:

$$\mathrm{Tr}(e^{-(H_{tb}+H_C)\beta}) \approx \mathrm{Tr}(e^{-H_{tb}\delta} I e^{-H_C\delta} I e^{-H_{tb}\delta} I e^{-H_C\delta} I .....)$$

Hubbard-Stratonovich transformation:

$$\int \prod d\varphi_x \exp\left(-\frac{1}{2}\sum_{x,y}\varphi_x V^{-1}_{x,y}\varphi_y - i\sum_x \varphi_x Q_x\right) \cong \exp\left(-\frac{1}{2}\sum_{x,y} Q_x V_{x,y} Q_y\right)$$

Final expression for Euclidean propagator:

$$g(x,y,\tau) = \mathrm{Tr}\left(\hat{a}^+_x e^{-\hat{H}\tau}\hat{a}_y e^{-\hat{H}(\beta-\tau)}\right) =$$

$$= \int \prod_{\varsigma} d\varphi^{(t)}_x M^{-1}_{x,y,t_0,t_0+\tau} e^{-S_{Hubbard}} \det(MM^+)$$

$$S_{Hubbard} = \frac{\delta}{2}\sum_{x,y,t}\varphi_{x,t} V^{-1}_{x,y}\varphi_{y,t}$$

Mass term and susceptibility (1)

Standard in Lattice QCD: introduction of small mass term and zero mass extrapolation

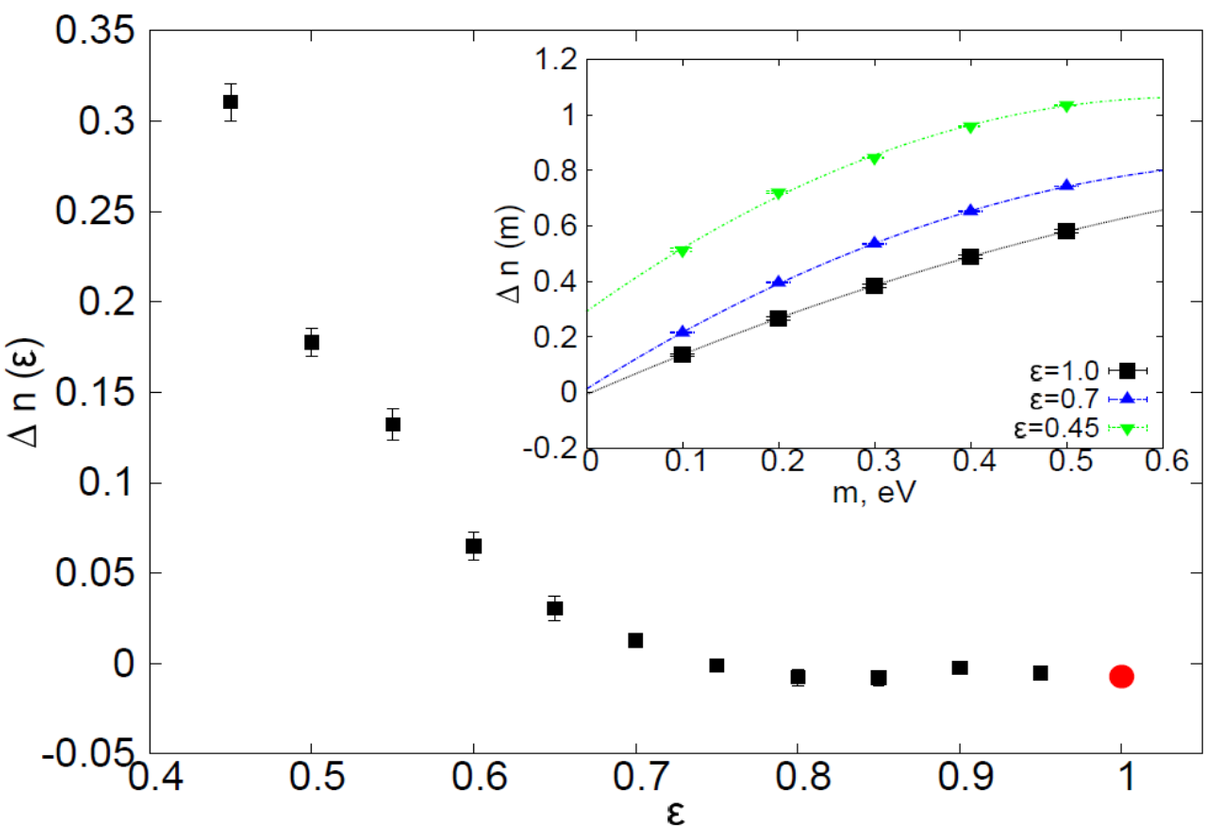
$$\sum_{x,y,t,t'} \psi^+_{x,t} M_{x,y,t,t'} \psi_{y,t'} = \sum_{n=0}^{N_t-1} \Bigg[\sum_x \psi^+_{x,2n}(\psi_{x,2n} - \psi_{x,2n+1}) +$$

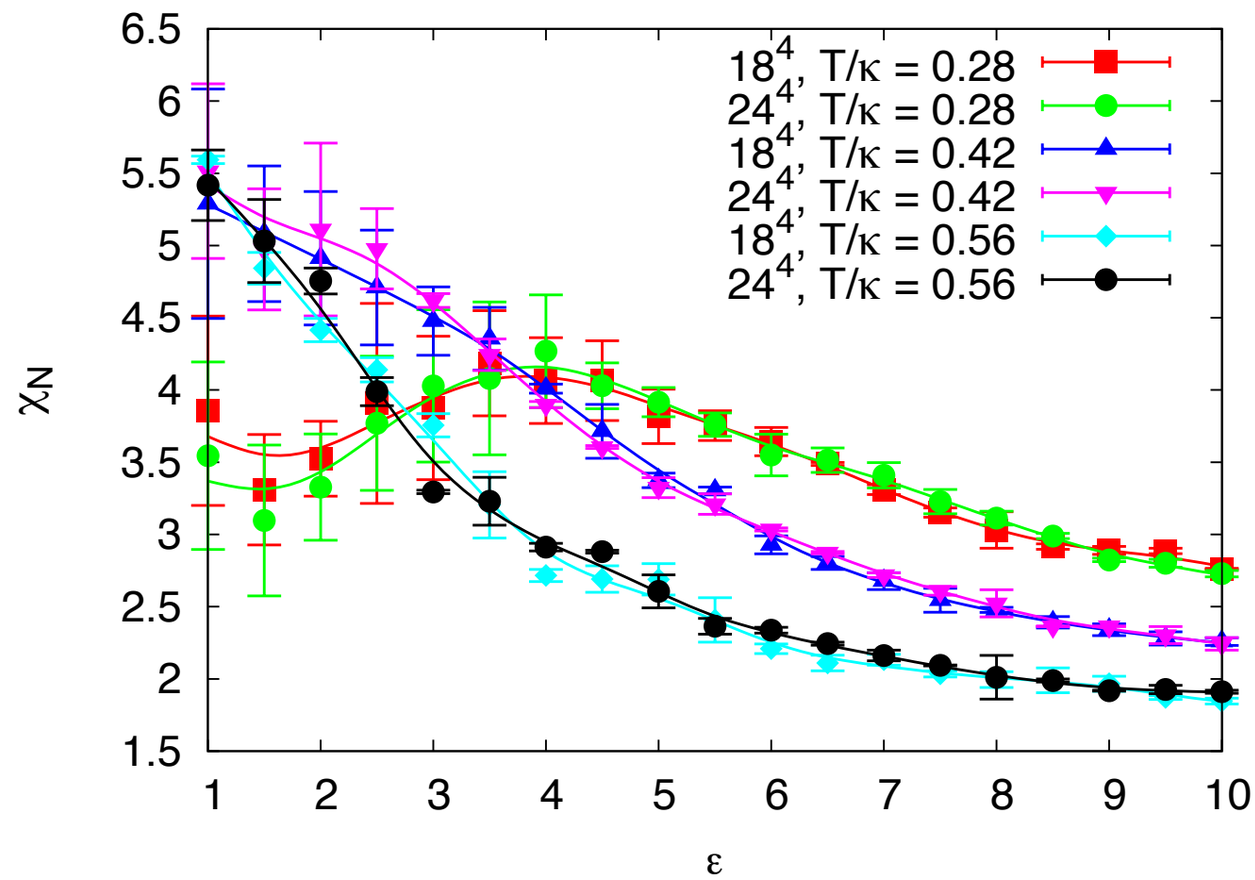
$$+ \sum_x \psi^+_{x,2n+1}\psi_{x,2n+1} - \delta\kappa \sum_{<x,y>} \left(\psi^+_{x,2n}\psi_{y,2n+1} + \psi^+_{y,2n}\psi_{x,2n+1}\right) +$$

$$+ m\delta \sum_{1st\ subLat} \psi^+_{x,2n}\psi_{x,2n+1} - m\delta \sum_{2d\ subLat} \psi^+_{x,2n}\psi_{x,2n+1} - \sum_x e^{-i\delta\phi_{x,2n+1}} \psi^+_{x,2n+1}\psi_{x,2n+2} \Bigg]$$

For antiferromagnetic phase transition mass term is equal for fermions and holes, thus $M_{el.} = M^*_{h.}$

Mass term and susceptibility (2)





$$\langle \Delta n_{AFM} \rangle = \frac{1}{N} \langle \sum_{x \in A} (\hat{a}^\dagger_{x,\uparrow} \hat{a}_{x,\uparrow} - \hat{a}^\dagger_{x,\downarrow} \hat{a}_{x,\downarrow}) - \sum_{x \in B} (\hat{a}^\dagger_{x,\uparrow} \hat{a}_{x,\uparrow} - \hat{a}^\dagger_{x,\downarrow} \hat{a}_{x,\downarrow}) \rangle$$

$$\chi \sim \langle \Delta^2 \rangle - \langle \Delta \rangle^2$$

arXiv:1304.3660

arXiv:1206.0619

Problem with different orders

$$\langle \Delta n_{AFM} \rangle = \frac{1}{N} \langle \sum_{x \in A} (\hat{a}^\dagger_{x,\uparrow} \hat{a}_{x,\uparrow} - \hat{a}^\dagger_{x,\downarrow} \hat{a}_{x,\downarrow}) - \sum_{x \in B} (\hat{a}^\dagger_{x,\uparrow} \hat{a}_{x,\uparrow} - \hat{a}^\dagger_{x,\downarrow} \hat{a}_{x,\downarrow}) \rangle$$

- different signes

$$\langle \Delta n_{CDW} \rangle = \frac{1}{N} \langle \sum_{x \in A} (\hat{a}^\dagger_{x,\uparrow} \hat{a}_{x,\uparrow} + \hat{a}^\dagger_{x,\downarrow} \hat{a}_{x,\downarrow}) - \sum_{x \in B} (\hat{a}^\dagger_{x,\uparrow} \hat{a}_{x,\uparrow} + \hat{a}^\dagger_{x,\downarrow} \hat{a}_{x,\downarrow}) \rangle$$

$$\sum_{x,y,t,t'} \psi^+_{x,t} M_{x,y,t,t'} \psi_{y,t'} = \sum_{n=0}^{N_t-1} \Bigg[\sum_x \psi^+_{x,2n} (\psi_{x,2n} - \psi_{x,2n+1}) +$$

$$+ \sum_x \psi^+_{x,2n+1} \psi_{x,2n+1} - \delta\kappa \sum_{<x,y>} \left(\psi^+_{x,2n} \psi_{y,2n+1} + \psi^+_{y,2n} \psi_{x,2n+1} \right) +$$

$$+ m\delta \sum_{1st\ subLat} \psi^+_{x,2n} \psi_{x,2n+1} - m\delta \sum_{2d\ subLat} \psi^+_{x,2n} \psi_{x,2n+1} - \sum_x e^{-i\delta\phi_{x,2n+1}} \psi^+_{x,2n+1} \psi_{x,2n+2} \Bigg]$$

Sign of CDW mass term is different for electrons and holes.

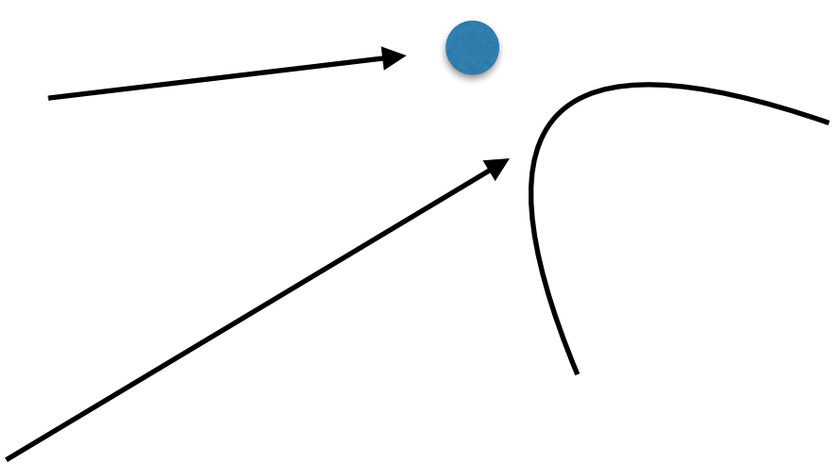
Role of mass term in Hybrid Monte Carlo

We evolve Hubbard field according to artificial Hamiltonian:

$$\mathcal{H} = \sum_{x,t} \frac{p_{x,t}^2}{2} + S(\{\varphi\})$$

$$S(\{\varphi_x^{(t)}\}) = S_{Hubbard} + \ln\det(M(\{\varphi_x^{(t)}\})M^+(\{\varphi_x^{(t)}\}))$$

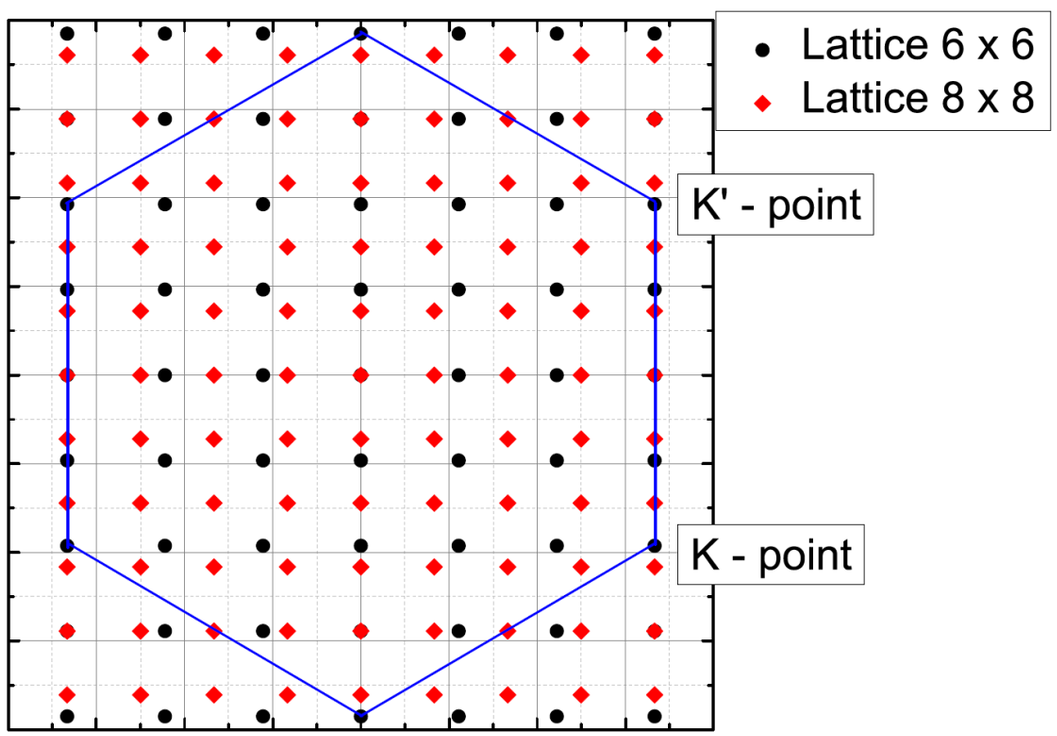
If one-particle Hamiltonian has zero modes, we are not safe from having zero modes of fermonic operator M in presence of interaction



Algorithm experiences difficulties in the vicinity of zero modes

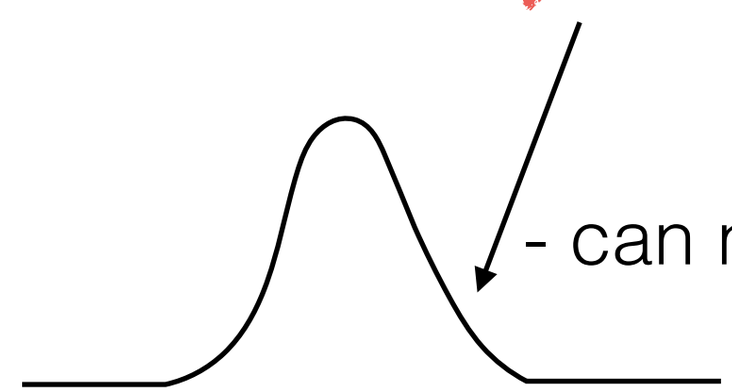
Geometric mass

If lattice is finite, Dirac points can fall somewhere in between lattice momenta



Since symmetry is preserved, order parameter is always zero!

$$\chi \sim \langle \Delta^2 \rangle - \cancel{\langle \Delta \rangle}^2$$



- can not fall down

Calculation of susceptibility is also senseless

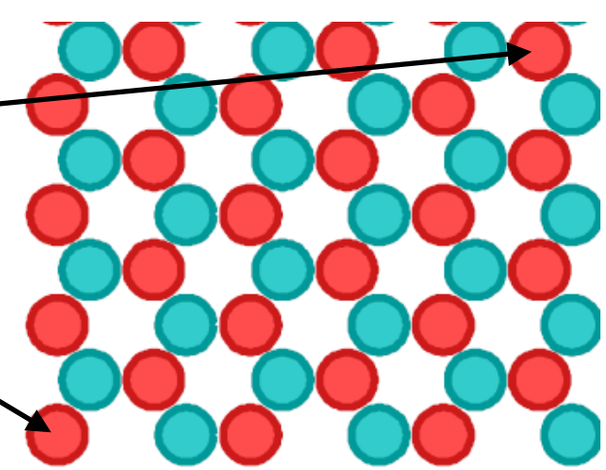
Finite-size scaling of order parameter (1)

$$\hat{S}_x^{(i)} = \frac{1}{2}(\hat{a}^\dagger_{x,\uparrow},\, \hat{a}^\dagger_{x,\downarrow})\sigma_i \begin{pmatrix} \hat{a}_{x,\uparrow} \\ \hat{a}_{x,\downarrow} \end{pmatrix}$$

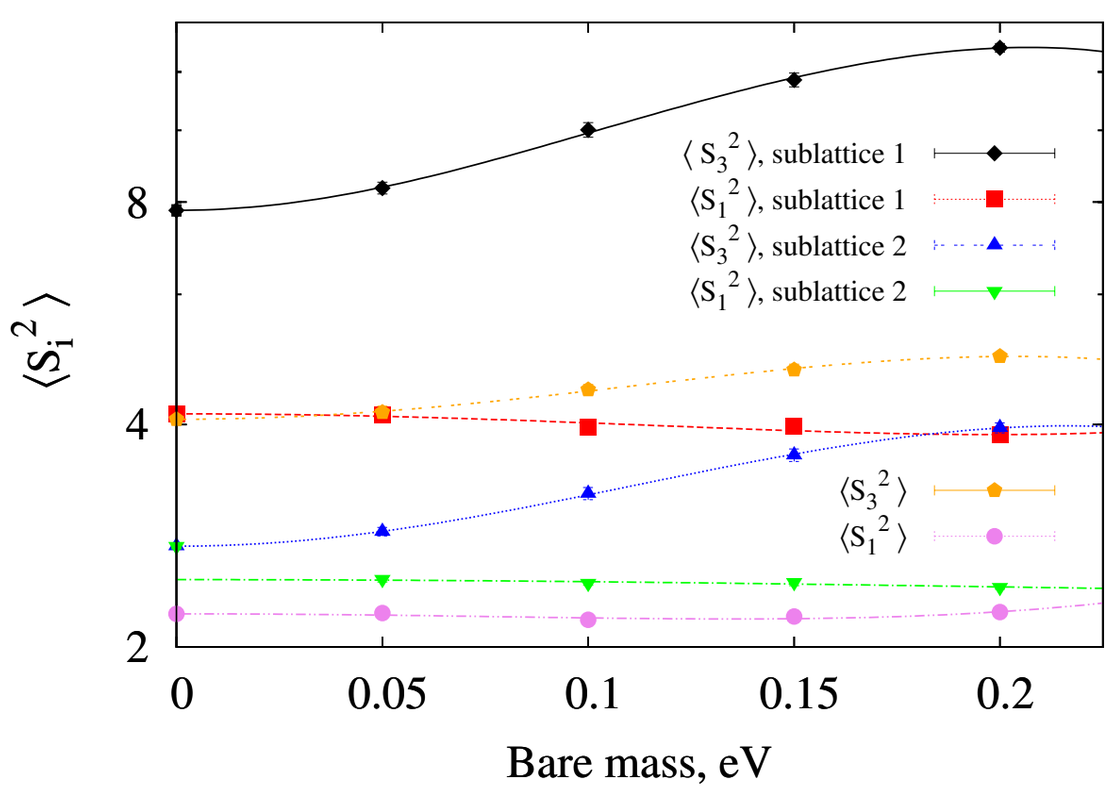
$$\langle S^{(i)} \rangle = \sqrt{\frac{\langle \left(\sum_{x=(1,\xi)} \hat{S}_x^{(i)} \right)^2 \rangle + \langle \left(\sum_{x=(2,\xi)} \hat{S}_x^{(i)} \right)^2 \rangle}{L^4}}$$

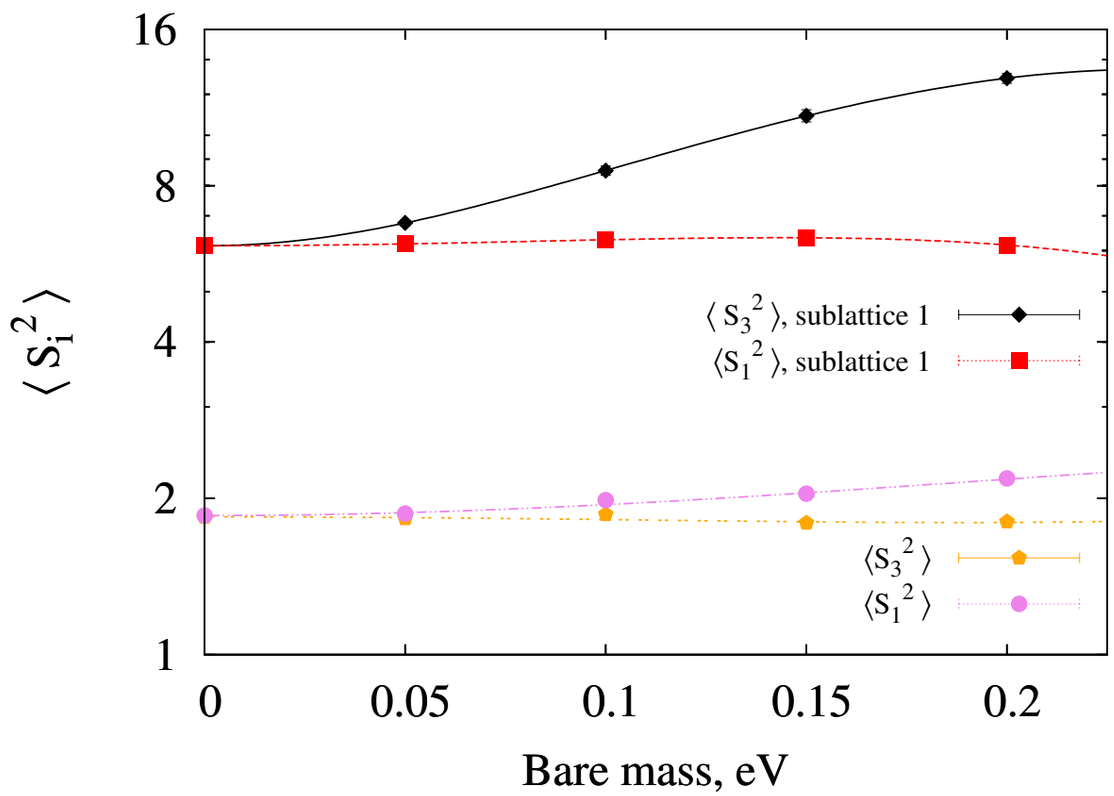
Finite value of $\langle S^{(i)} \rangle$ in thermodynamic limit is equivalent to nonzero correlation of spins at infinity (ordered phase).

<SxSy> ~ C at one sublattice even for infinitely distant sites

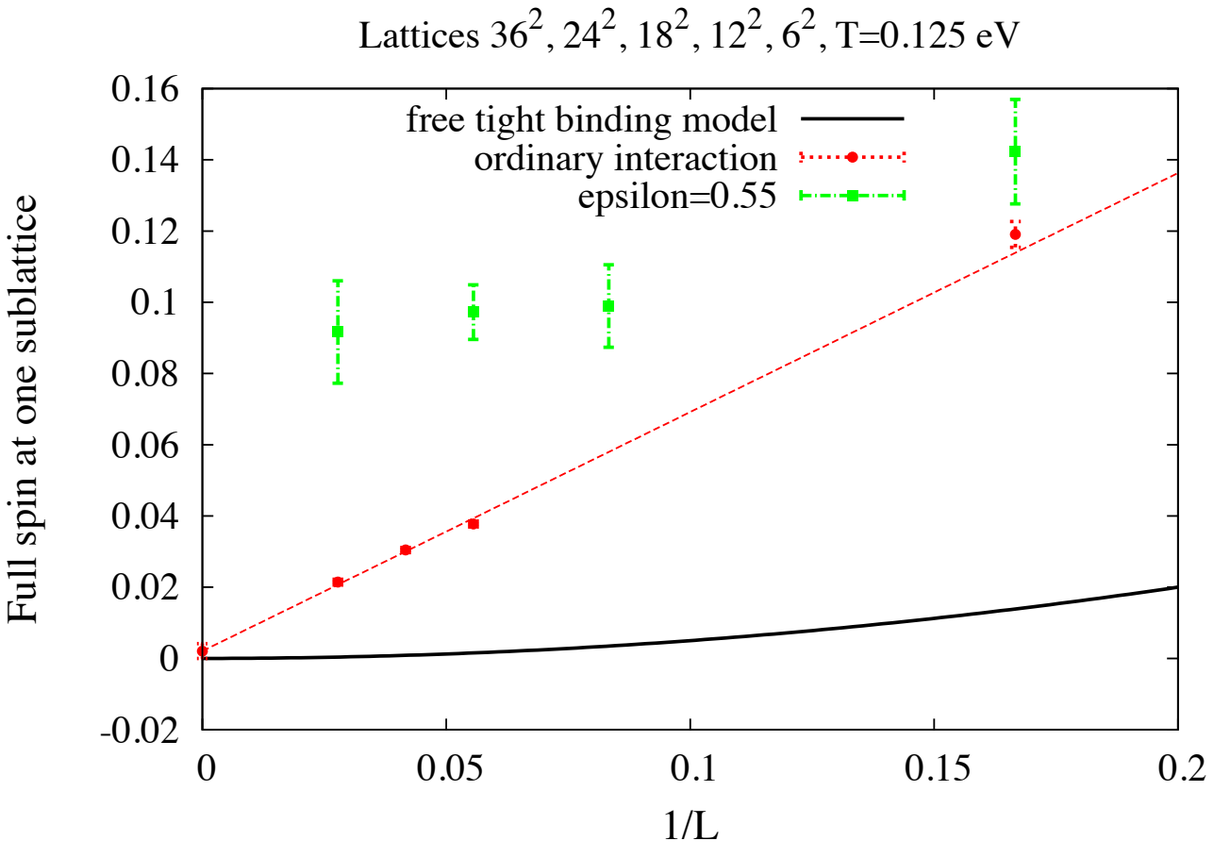


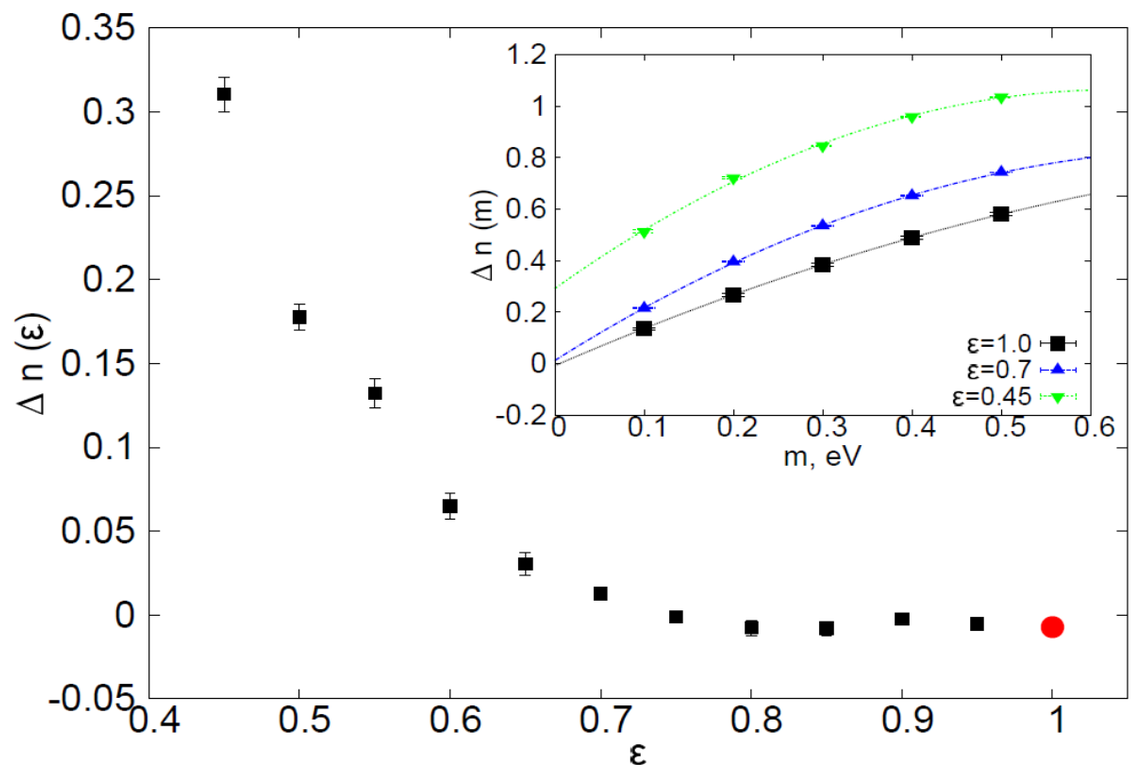
Finite-size scaling of order parameter (2)





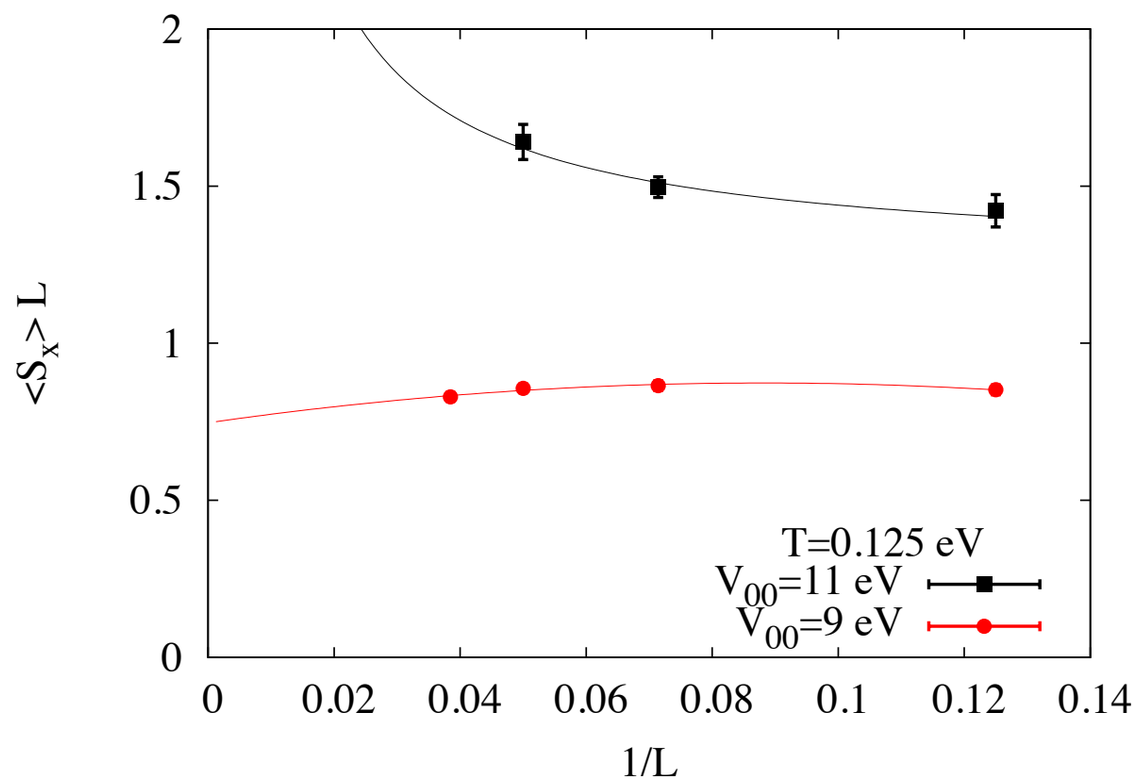
Finite-size scaling of order parameter (3)



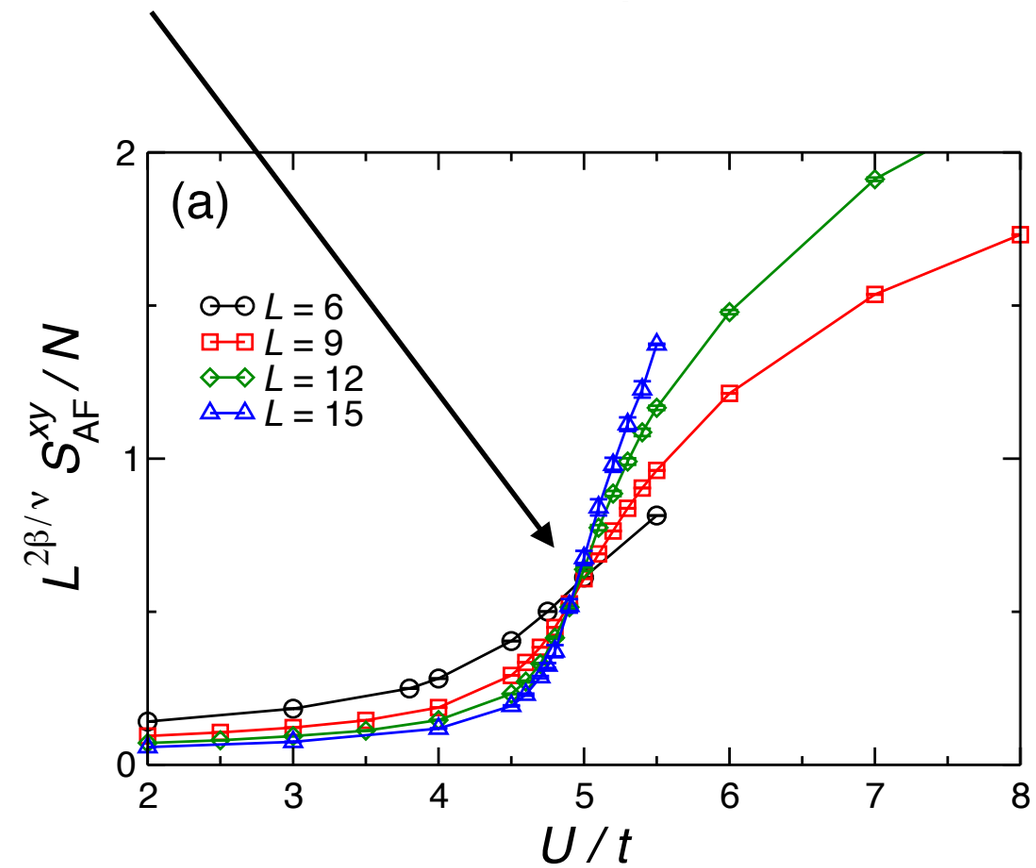


Finite-size scaling of order parameter (4)

Exact location of the phase transition point

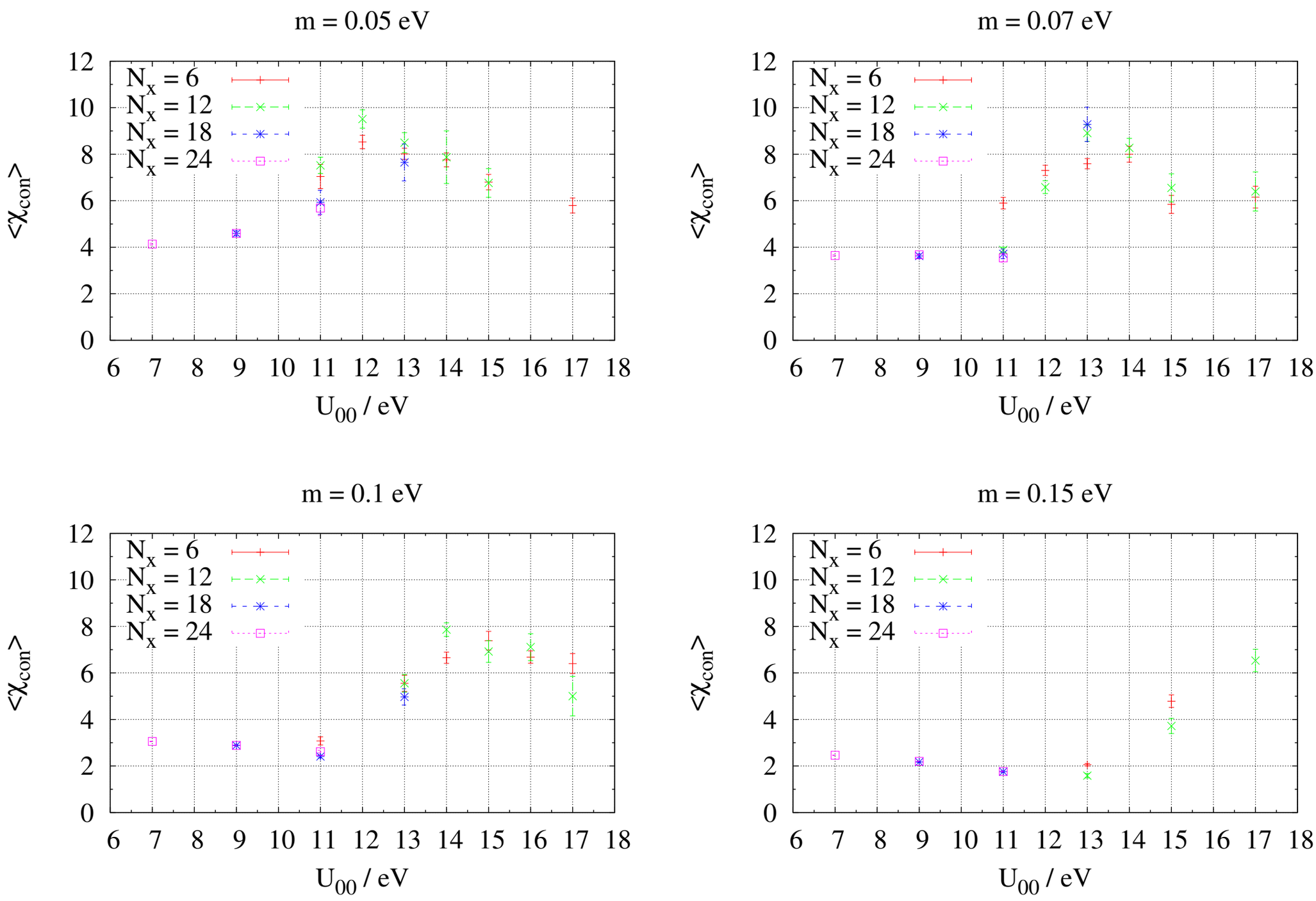


Example calculation of pure Hubbard model on hexagonal lattice

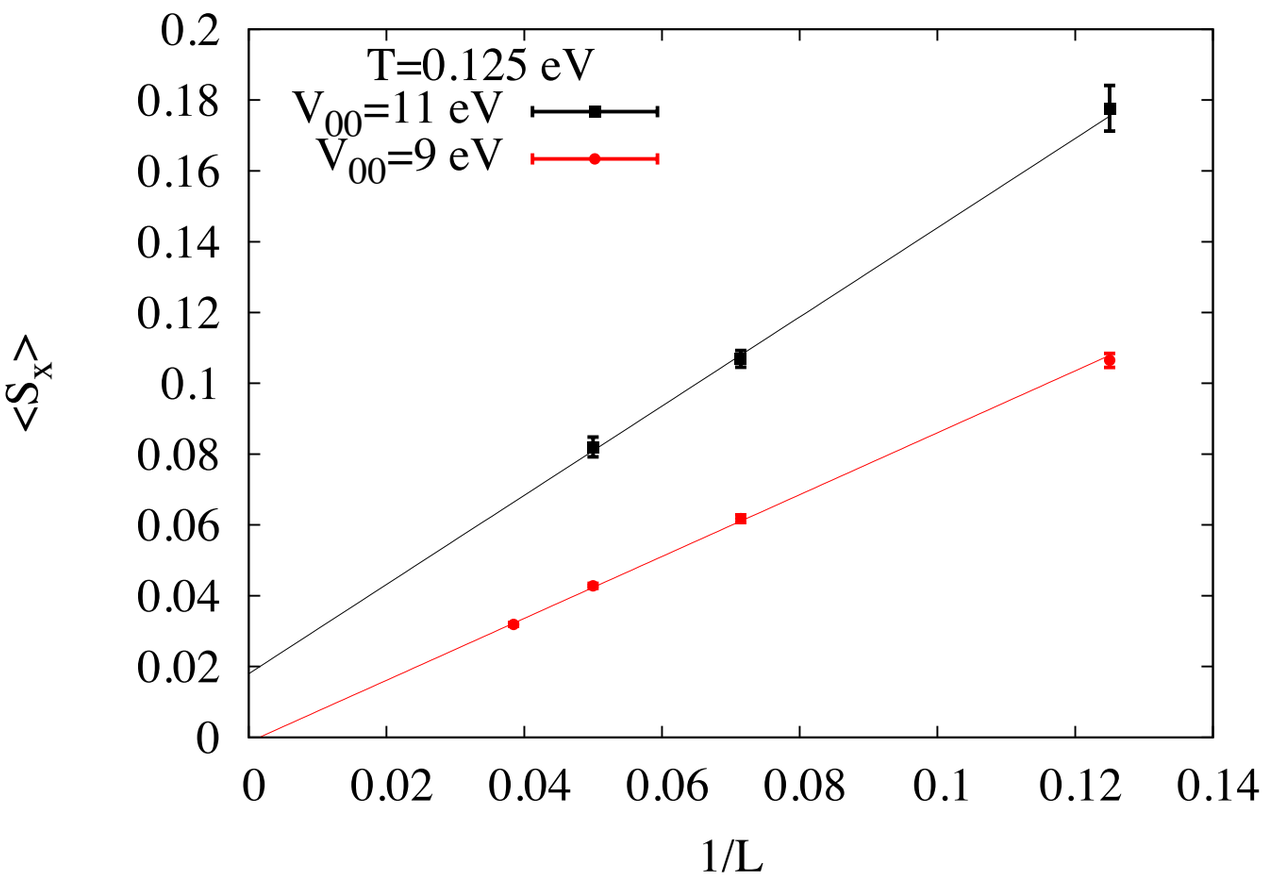


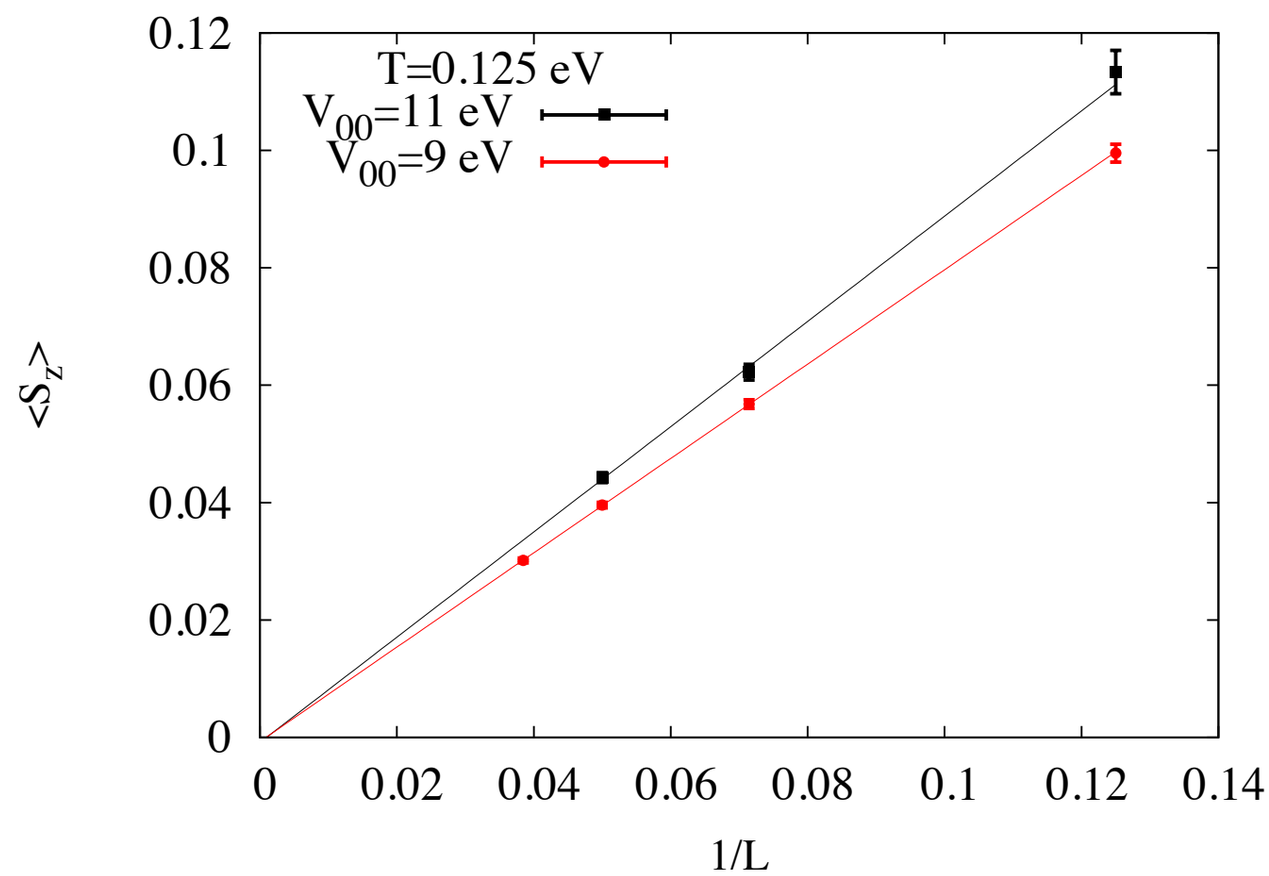
Kane-Meld-Hubbard model: arXiv: 1111.3949

Hubbard model simulations (only on-site interaction)



Hubbard model simulations (only on-site interaction)





Transition in between V_{00}=9 eV and 11 eV

Connection between time discretization and spin symmetry (1)

$$\langle \left(\hat{S}_x^{(1)} \hat{S}_y^{(1)} \right) \rangle |_{\substack{x=(1,\xi) \\ y=(2,\zeta)}} = -\frac{1}{4} \left(|g(x,y)|^2 + |g(y,x)|^2 \right)$$

$$\langle \left(\hat{S}_x^{(3)} \hat{S}_y^{(3)} \right) \rangle |_{\substack{x=(1,\xi) \\ y=(2,\zeta)}} = \frac{1}{4} \left((1 - 2\mathrm{Re}\, g(x,x) - 2\mathrm{Re}\, g(y,y) + 2\mathrm{Re}\, (g(x,x)g(y,y)) + 2\mathrm{Re}\, (g(x,x)^\dagger g(y,y)) - g(x,y)g(y,x)) \right)$$

$$g(x,y) = \langle \hat{a}_{x,\uparrow} \hat{a}_{y,\uparrow}^\dagger \rangle$$

At neutrality point *g(x,x)=0.5* (ideally), thus two correlators should be equivalent

Connection between time discretization and spin symmetry (2)

Lattice operator in momentum space:

$$M(\omega,\vec{k}) = \Delta\tau \begin{pmatrix} \frac{1-e^{-i\omega\Delta\tau}}{\Delta\tau} & \kappa S(\vec{k})e^{-i\omega\Delta\tau} \\ \kappa S^*(\vec{k})e^{-i\omega\Delta\tau} & \frac{1-e^{-i\omega\Delta\tau}}{\Delta\tau} \end{pmatrix} \qquad S(\vec{k}) = \sum_{i=1}^{3} e^{i\vec{\delta}_i\vec{k}}$$

In continuous time and zero temperature: $\dfrac{1-e^{-i\omega\Delta\tau}}{\Delta\tau} \to i\omega$

$$M^{-1}(\omega,\vec{k}) = \frac{-1}{\omega^2+\kappa^2|S|^2} \begin{pmatrix} i\omega & -\kappa S^* \\ -\kappa S & i\omega \end{pmatrix}$$

$$M^{-1}_{x,t,x,t} = \frac{1}{2\pi V_k}\int d\omega \sum_{\vec{k}} \frac{i\omega}{-\omega^2-\kappa^2|S|^2} = \frac{1}{2}$$

$$\int d\omega \frac{i\omega}{-\omega^2-\kappa^2|S|^2} = \lim_{\varepsilon\to+0}\int d\omega \frac{i\omega}{-\omega^2-\kappa^2|S|^2} e^{i\omega\varepsilon} = \frac{1}{2}$$

In discrete time there are corrections to the integral of the order $\Delta\tau^2$

Connection between time discretization and spin symmetry (3)

In principle, it's possible to avoid time discretization for free fermions:

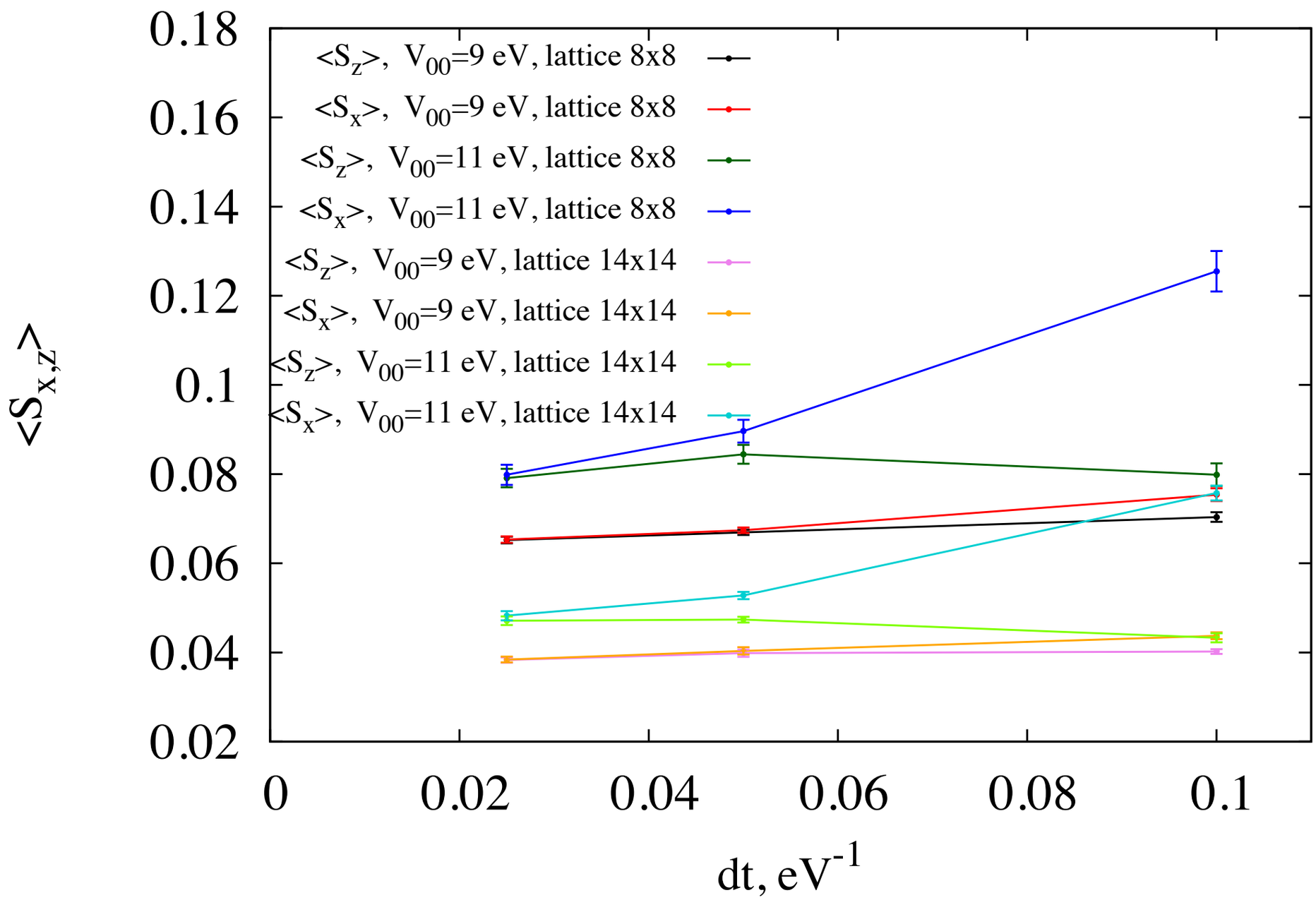
$$\sum_{x,y,t,t'} \psi^+_{x,t} M_{x,y,t,t'} \psi_{y,t'} = \sum_{n=0}^{N_t-1} \Bigg[\sum_x \psi^+_{x,2n}(\psi_{x,2n} - \psi_{x,2n+1}) +$$

$$+ \sum_x \psi^+_{x,2n+1}\psi_{x,2n+1} - \delta\kappa \sum_{<x,y>} \left(\psi^+_{x,2n}\psi_{y,2n+1} + \psi^+_{y,2n}\psi_{x,2n+1}\right) +$$

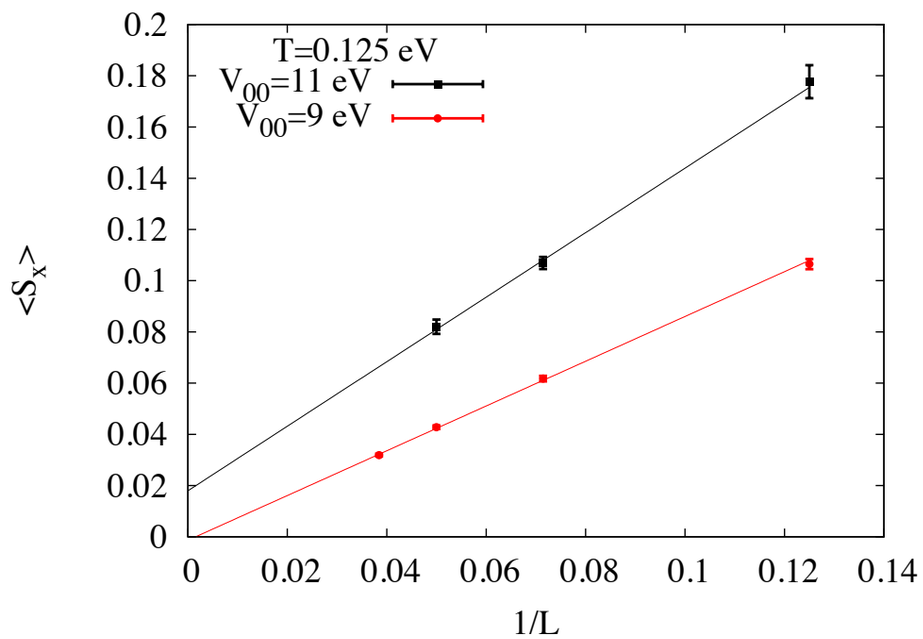
$$+ m\delta \sum_{1st\ subLat} \psi^+_{x,2n}\psi_{x,2n+1} - m\delta \sum_{2d\ subLat} \psi^+_{x,2n}\psi_{x,2n+1} - \sum_x e^{-i\delta\phi_{x,2n+1}} \psi^+_{x,2n+1}\psi_{x,2n+2} \Bigg]$$

$$e^{-\Delta\tau H} \to 1 - \Delta\tau H$$

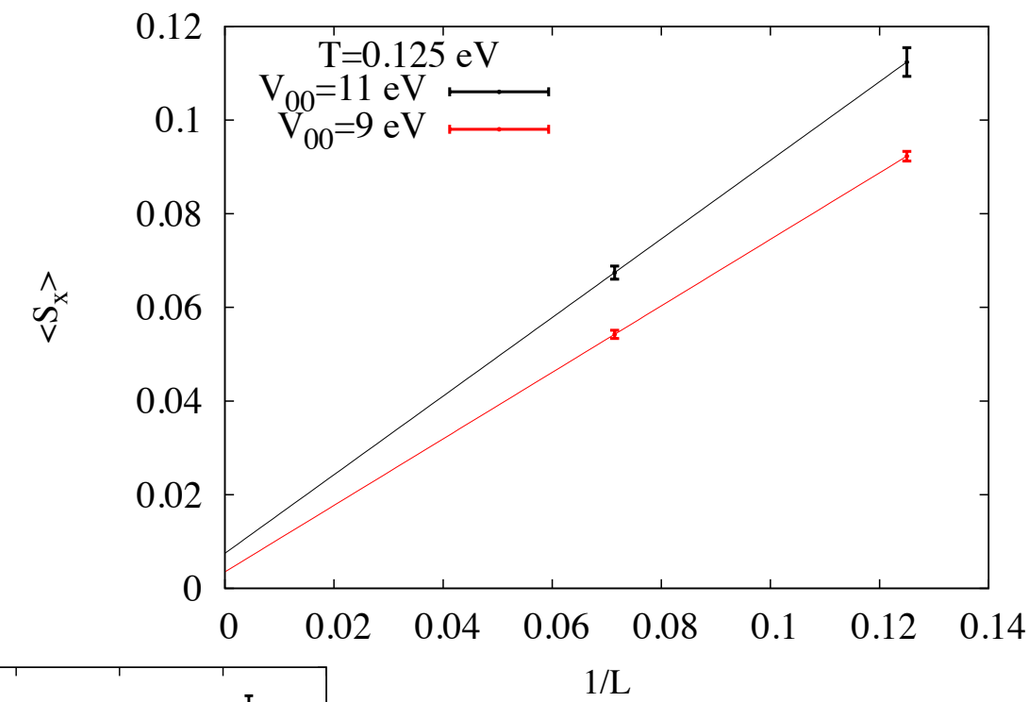
Zero time step extrapolation



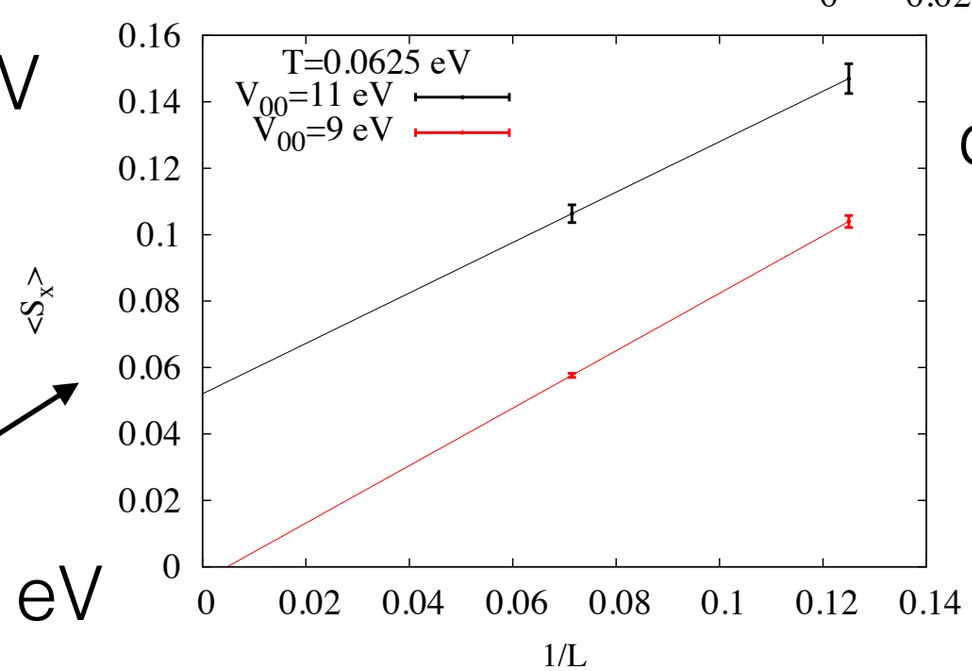
Influence of time discretization on physical results



dt=0.1, T=0.125 eV

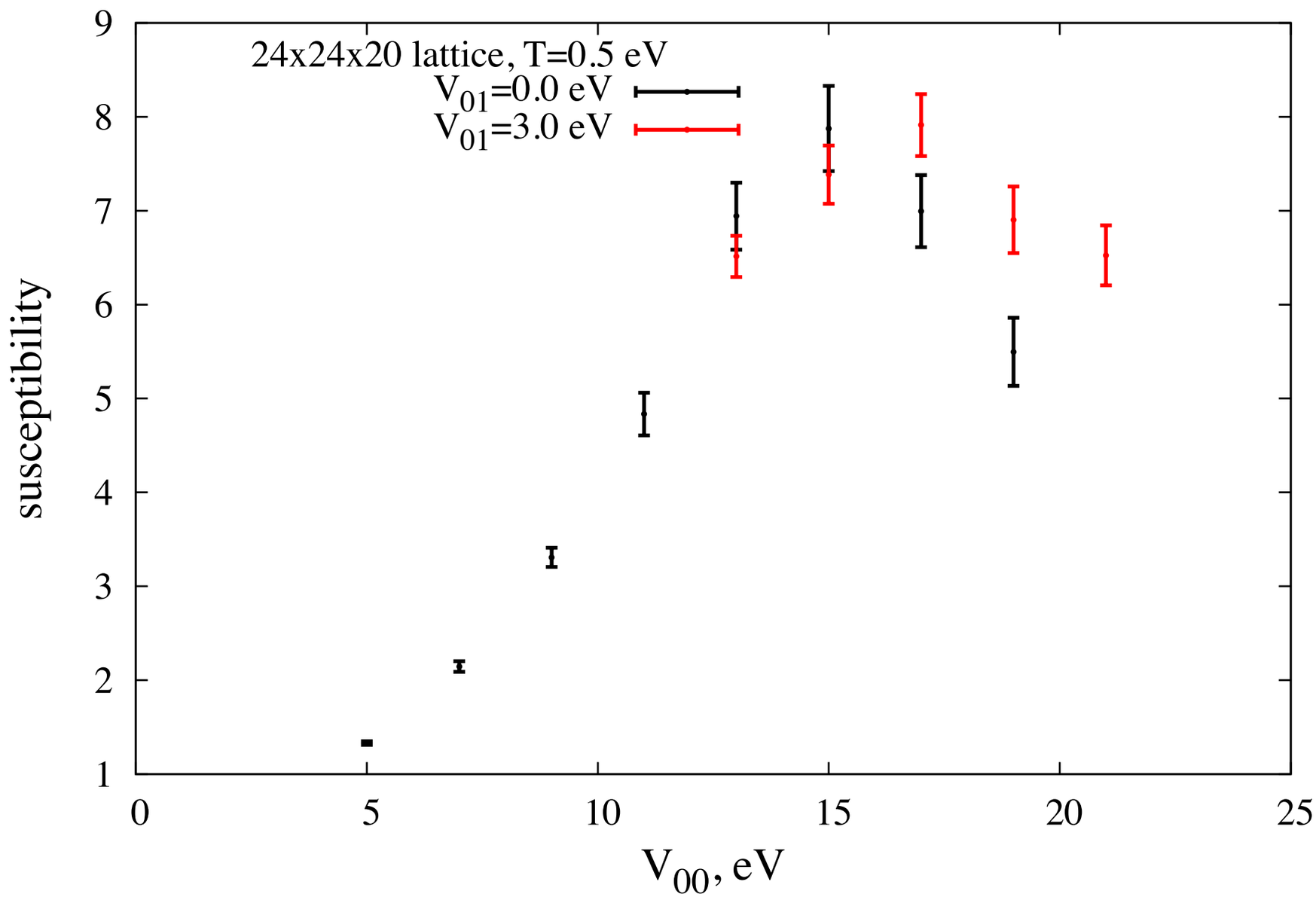


dt=0.025, T=0.125 eV

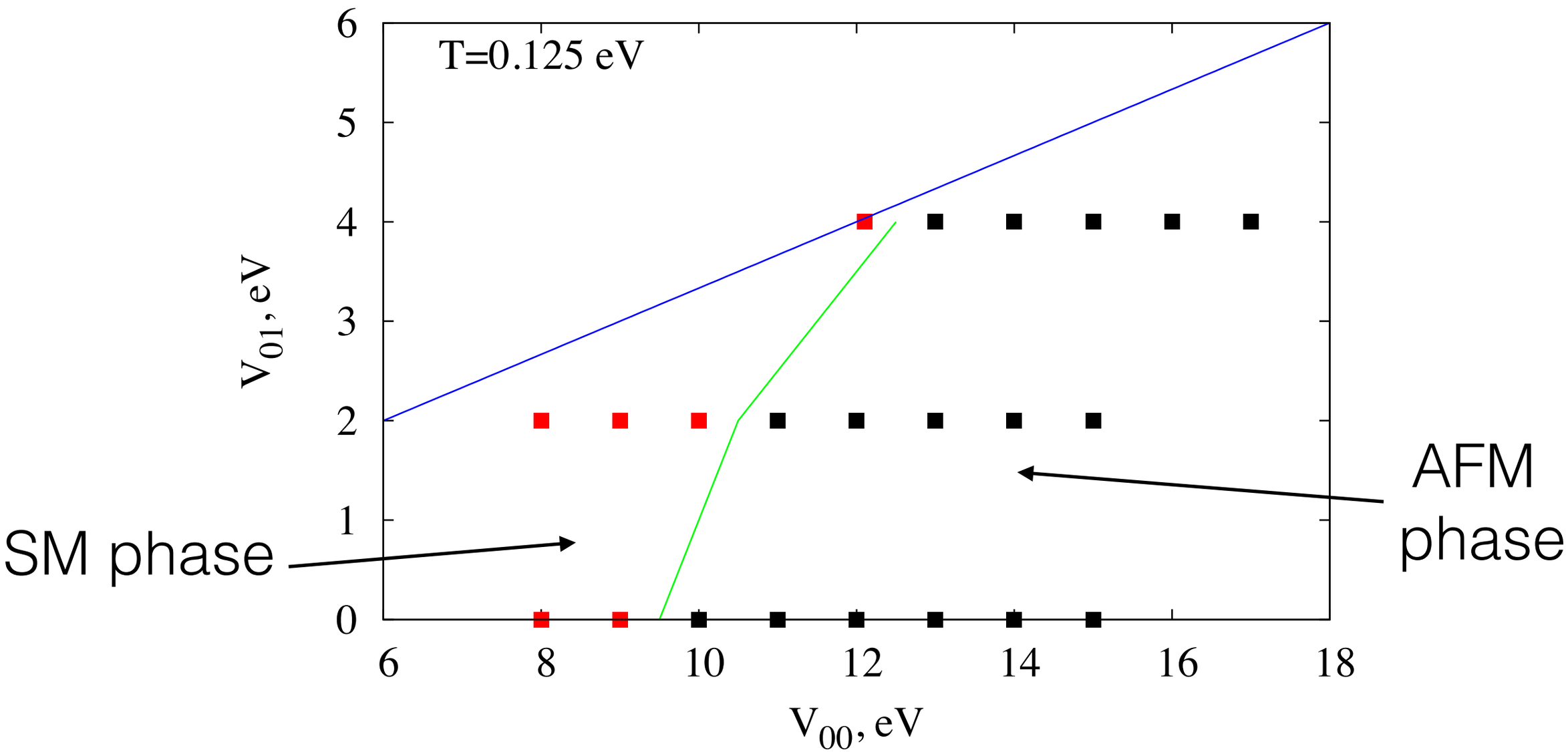


dt=0.025, T=0.0625 eV

High temperature phase diagram



Low temperature phase diagram



Conclusion

1) Preliminary results on the phase diagram for extended Hubbard model are presented. The line of AFM phase transition violates both V_{00}=const and V_{00}-V_{01}=const laws.
2) Several ways to identify phase transition are discussed. Standard lattice techniques doesn't work well and we should employ finite size scaling of squared order parameter.
3) Special attention should be payed to lattice artifacts connected with discretization of euclidean time.