Direct detection of metal-insulator phase transitions using modified Backus-Gilbert method

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HMC for condensed matter systems

We should compare with BSS-QMC method where the mapping into complicated classical spin model is used instead of Hubbard-Stratonovich transformation (Hirsch, 1984):

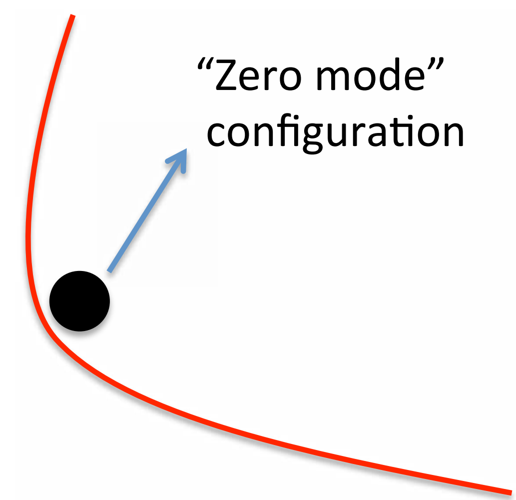
$$\hat{n}_{\uparrow}\hat{n}_{\downarrow} \rightarrow \sigma = \pm 1$$

The comparison is still ongoing project, but some outcome is already clear:

- BSS-QMC is faster for small lattices (< ≈ 18x18x100) for pure on-site interaction.
- for Coulomb interaction, HMC is definitely faster for almost all lattice sizes.

However, some modifications are needed:

- Simulations in exactly chiral regime (m=0)
- Increasing flexibility (different lattices, etc)



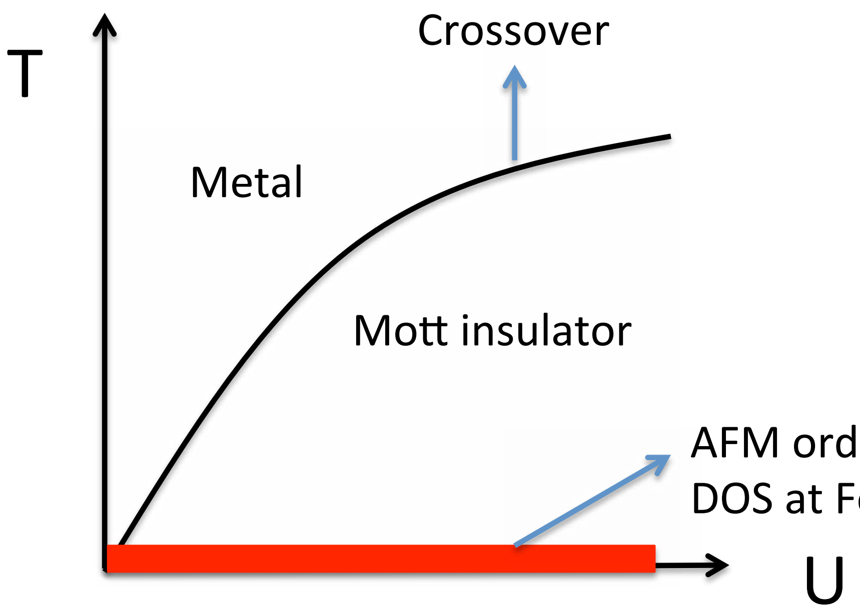
- Alternative methods to identify the phase transitions

Motivation (1)

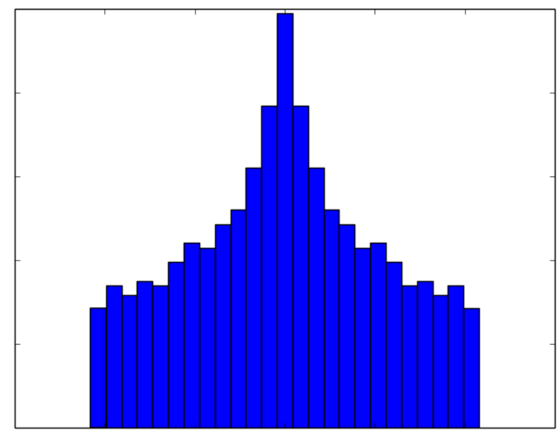
Study of metal-insulator transition is the most obvious task for HMC in condensed matter physics.

Hubbard model on square lattice:

$$\hat{H} = -\kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle x,y \rangle} (\hat{c}^\dagger_{x,\sigma}\hat{c}_{y,\sigma} + \text{h.c.}) + U \sum_x (\hat{n}_{x\uparrow} - \frac{1}{2})(\hat{n}_{x\downarrow} - \frac{1}{2})$$



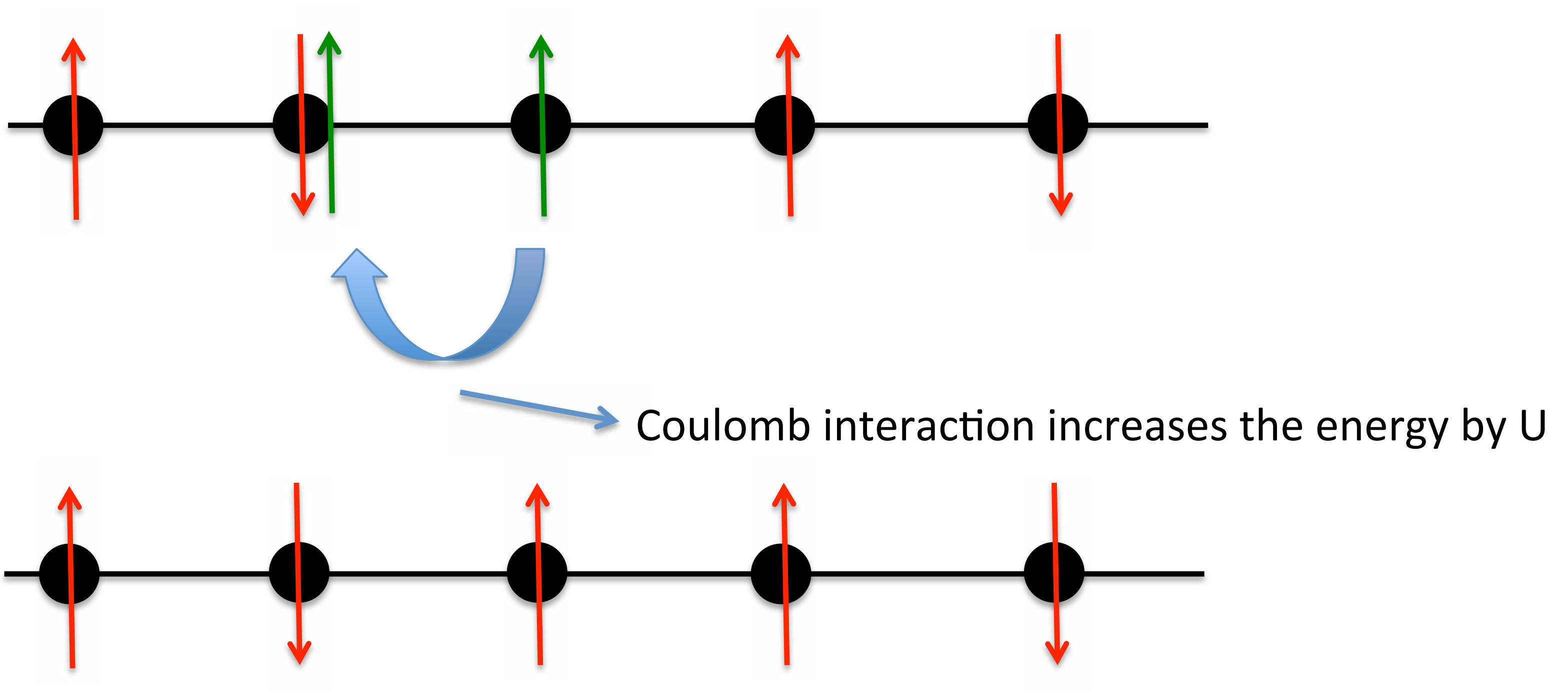
AFM order at zero temperature at any U due to divergent DOS at Fermi energy



The most recent calculation: T. Schäfer et. al. PRB 91, 125109 (2015)

Motivation (2)

Mott insulator: strong Coulomb on-site repulsion prevents the double occupancy of the lattice sites:

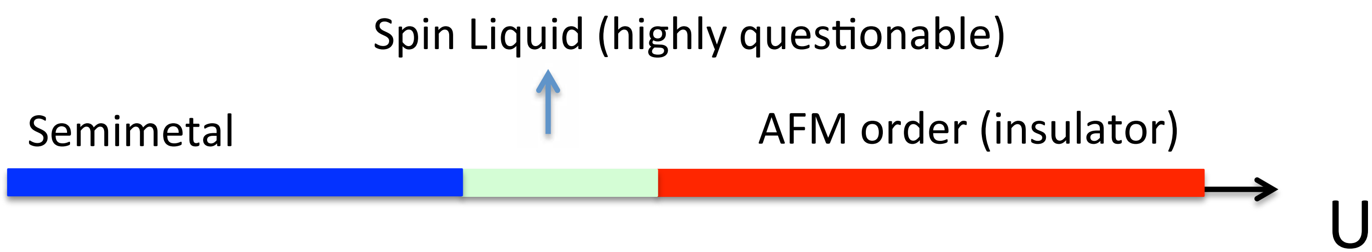


Electrons are localized in configuration space instead of being localized in momentum space. But it doesn't mean that the spin or charge is ordered! E.g. magnetization can be destroyed by temperature, frustration or just by long-range spin fluctuations.

Motivation (3)

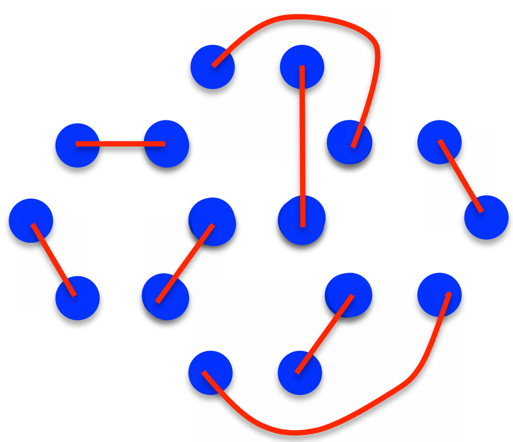
Things are even more tricky for the Hubbard model on hexagonal lattice.

Zero temperature phase diagram:



Probably contains the spin liquid phase: collection of dimers with no local order parameter.

$$|S=0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right)$$



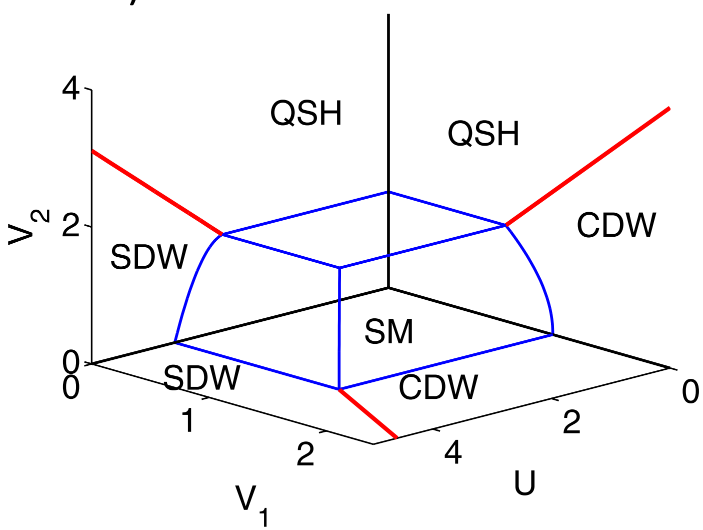
Nature 464, 847 (2010) (+)
PRL 107, 087204 (2011) (+)
PRB 84, 2015121 (2011) (+)
PRB 85, 235149 (2011) (+)
PRL 106, 100403 (2011) (+)
Sci. Rep. 2, 992 (2012) (-)
PRB 85, 115132 (2012) (+)
PRX 3, 031010 (2013) (-)

Motivation (4)

Another possibility is realized in extended Hubbard model: multiple phases including charge density wave, topological phases, etc.

$$\hat{H} = -\kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle x,y\rangle} \left(\hat{c}^\dagger_{x,\sigma}\hat{c}_{y,\sigma} + \mathrm{h.c.}\right) + U \sum_x \hat{q}_x^2 + V_1 \sum_{\langle x,y\rangle} \hat{q}_x \hat{q}_y + V_2 \sum_{\langle\langle x,y\rangle\rangle} \hat{q}_x \hat{q}_y$$

Example mean-field phase diagram for extended Hubbard model on hexagonal lattice: (PRL 100 (2008), 156401)



Standard calculation of susceptibility in simulations with mass term is often impossible.

Analytical continuation. Backus-Gilbert method

Main aim: the development of the method for analytic continuation, which involves as few assumptions about the spectral function as possible.

$$G(\tau) = \int_0^\infty d\omega K(\tau, \omega) A(\omega)$$

$$K(\tau, \omega) \equiv \frac{\cosh\left[\omega(\tau - \beta/2)\right]}{\cosh(\omega\beta/2)}$$

$$K(\tau, \omega) \equiv \frac{\sinh\left[\omega(\tau - \beta/2)\right]}{\cosh(\omega\beta/2)}$$

→ Density of States (DOS), possibly momentum-resolved:

$$A(\omega) = \mathrm{Im} G_R(\omega)/\pi$$

$$G(\tau) = \sum_x \langle M^{-1}_{x,\tau;x,0} \rangle_\phi$$

$$K(\tau, \omega) \equiv \frac{\omega \cosh\left[\omega(\tau - \beta/2)\right]}{\sinh(\omega\beta/2)}$$

→ Conductivity, obtained from current-current correlator

Basic ideas of the method

B. Brandt et. al. PRD, 92, 0945120 (2015)

Convolution of the spectral function with some resolution function:

$$\bar{A}(\omega_0) = \int_0^\infty d\omega \delta(\omega_0, \omega) A(\omega)$$

Method is linear:

$$\delta(\omega_0, \omega) = \sum_j q_j(\omega_0) K(\tau_j, \omega) \qquad \bar{A}(\omega_0) = \sum_j q_j(\omega_0) G(\tau_j)$$

Minimization of the width of the resolution function:

$$D \equiv \int_0^\infty d\omega (\omega - \omega_0)^2 \delta^2(\omega_0, \omega) \qquad \int_0^\infty d\omega \delta(\omega_0, \omega) = 1$$

$$q_j(\omega_0) = \frac{W^{-1}(\omega_0)_{j,k} R_k}{R_n W^{-1}(\omega_0)_{n,m} R_m}$$

$$W(\omega_0)_{j,k} = \int_0^\infty d\omega (\omega - \omega_0)^2 K(\tau_j, \omega) K(\tau_k, \omega)$$

$$R_n = \int_0^\infty d\omega K(\tau_n, \omega)$$

Regularization (1)

Regularization with the covariance matrix:

$$W(\omega_0)_{j,k} \to (1-\lambda)W(\omega_0)_{j,k} + \lambda C_{j,k}$$

Regularization during SVD decomposition of the kernel:

$$W = U\Sigma V^\top,\ UU^\top = VV^\top = \mathbf{1}$$

$$W^{-1} = VDU^\top,\ D = \mathrm{diag}(\sigma_1^{-1}, \sigma_2^{-1}, \ldots, \sigma_N^{-1})$$

$$D_{i,j} \to \tilde{D}_{i,j} = \delta_{ij}\frac{\sigma_i}{\sigma_i^2 + \lambda^2}$$

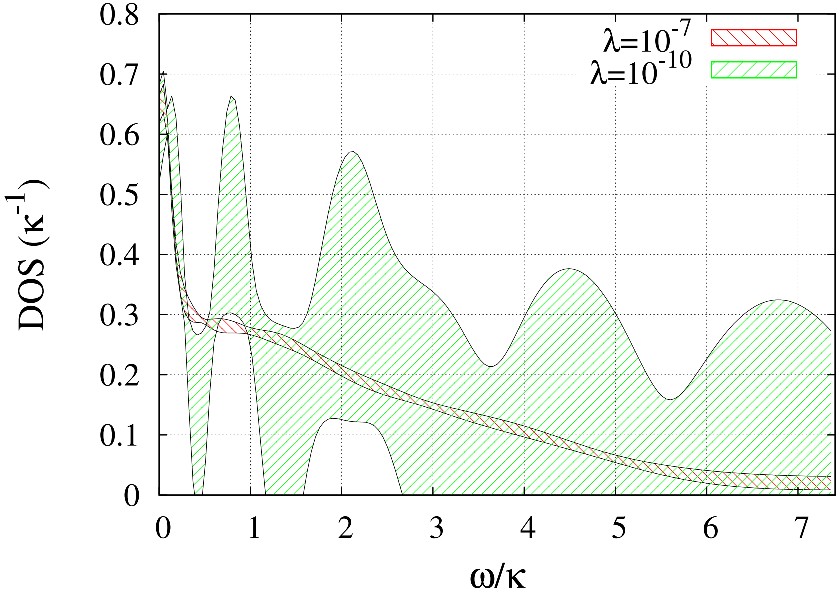
$$\tilde{D}_{i,j} = \delta_{ij}\frac{1}{\sigma_i + \lambda}$$

$$Ax = b$$

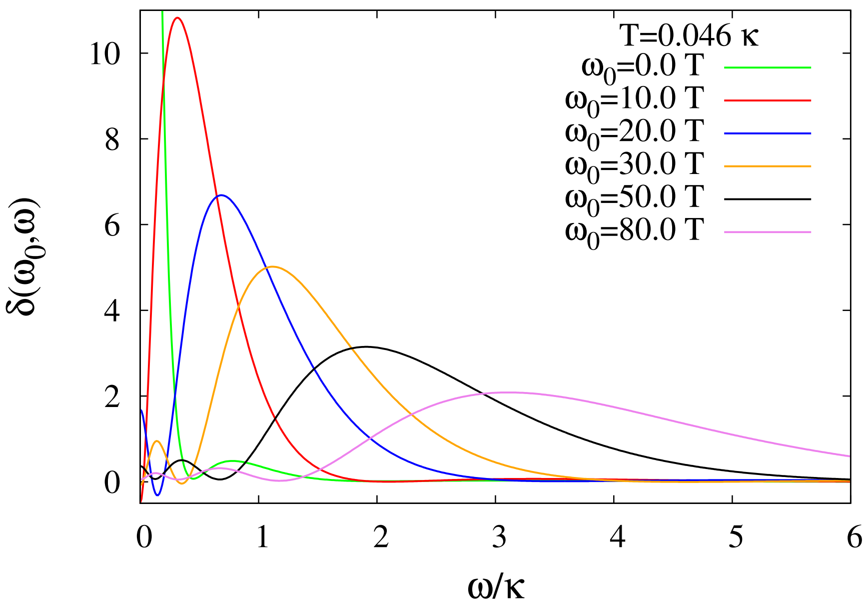
$$\min\left(\|Ax - b\|_2^2 + \|\Gamma x\|_2^2\right)$$

Regularization: How it works

Square Lattice Hubbard-Coulomb model, N_s=20.

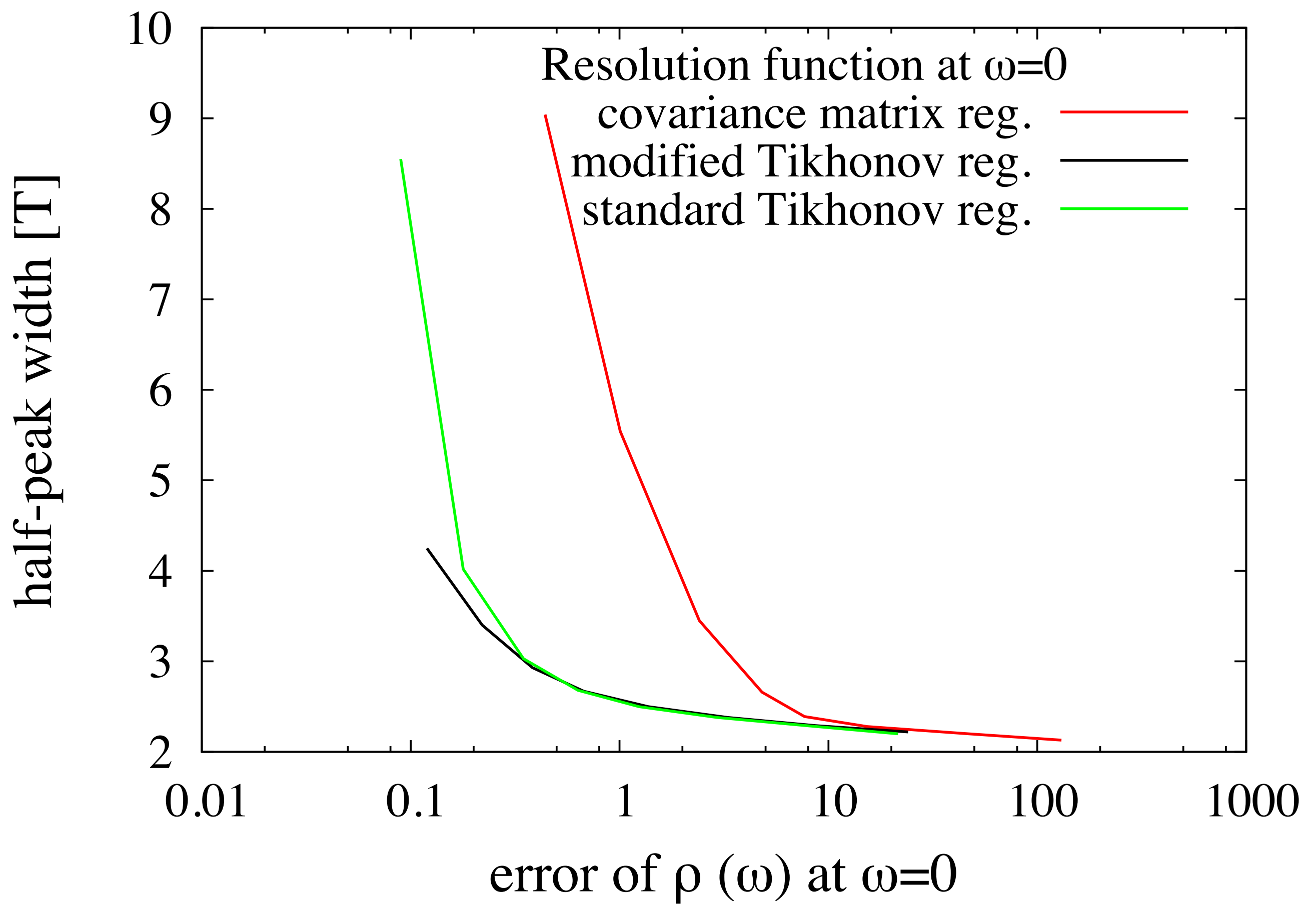


Density of States

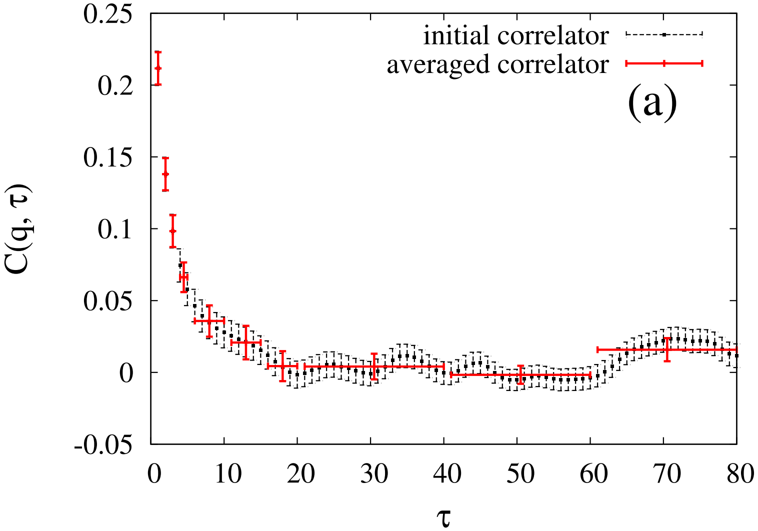


Resolution functions

Comparison of different regularizations



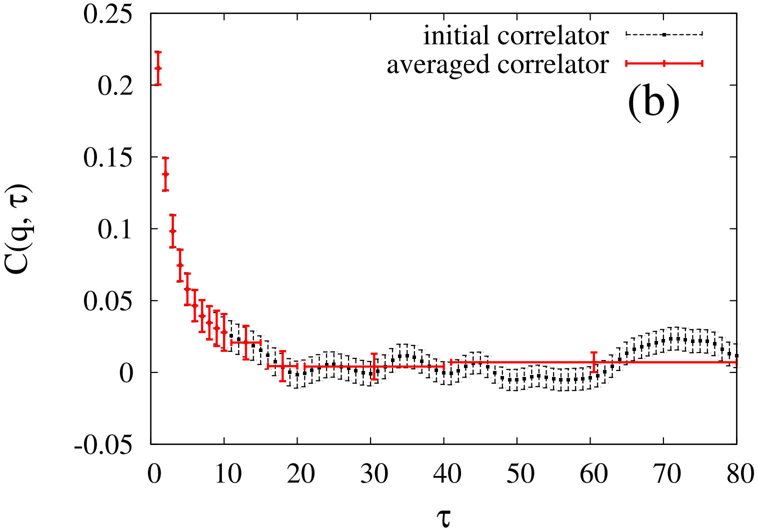
Regularization (2): averaging over time intervals

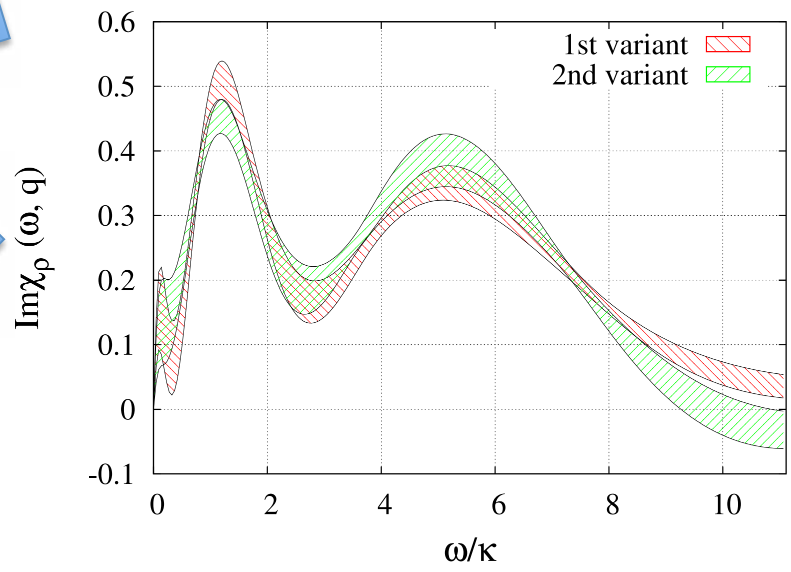


$$\{G(\tau_i), \Delta G(\tau_i);\ i = 0, 1, \ldots, N_\tau - 1\}$$

$$\{\tilde{G}(\tilde{\tau}_j), \Delta\tilde{G}(\tilde{\tau}_j);\ j = 1, \ldots, N_{\text{int}}\}$$

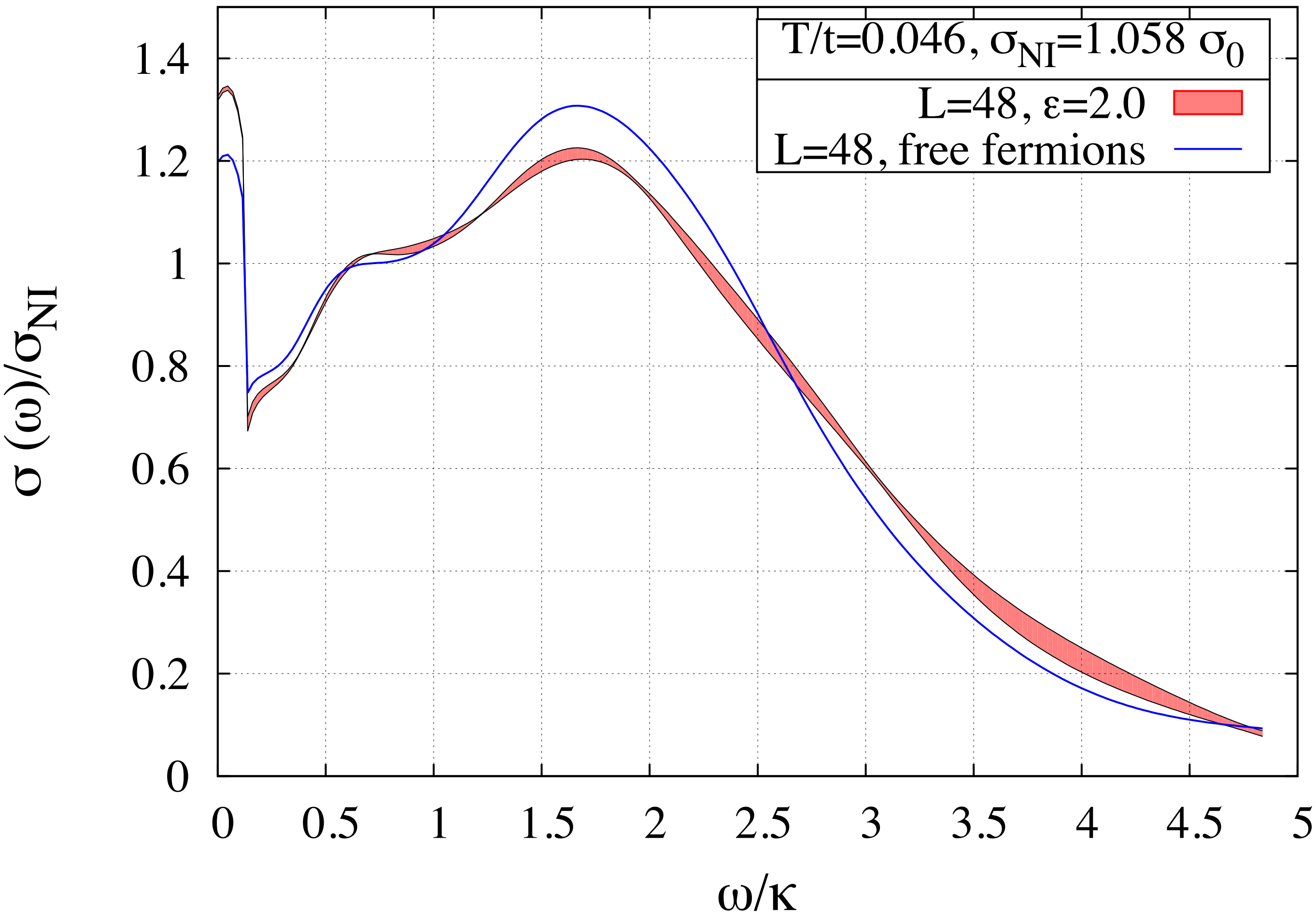
$$\tilde{G}(\tilde{\tau}_j) \equiv \frac{1}{\tilde{N}_j} \sum_{i=1}^{\tilde{N}_j} G(\tau_i^{(j)})$$





Example calculation: Graphene conductivity

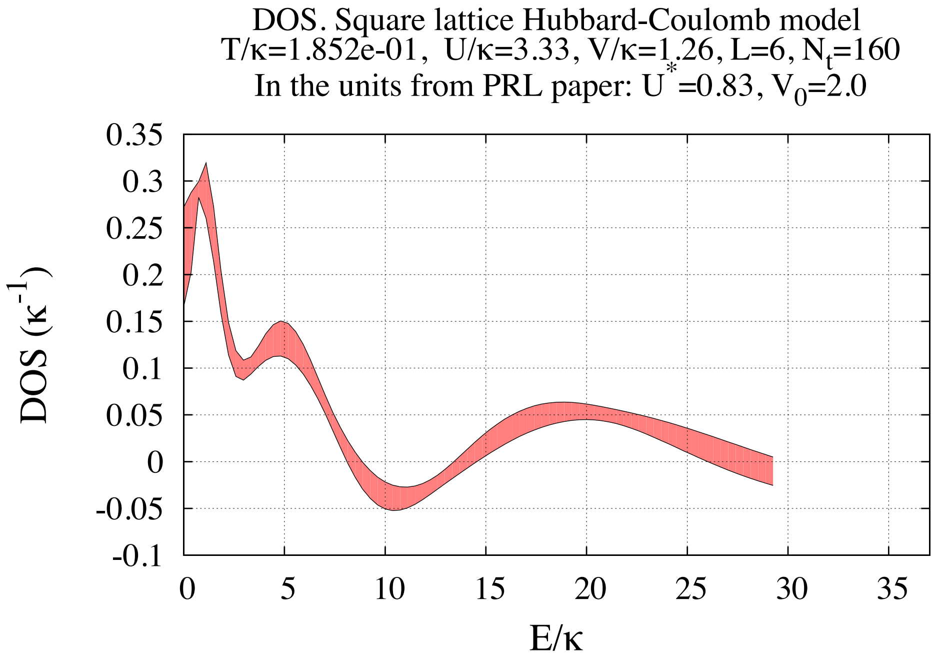
Hubbard-Coulomb model on hexagonal lattice, 48x48 lattice with N_t=80.

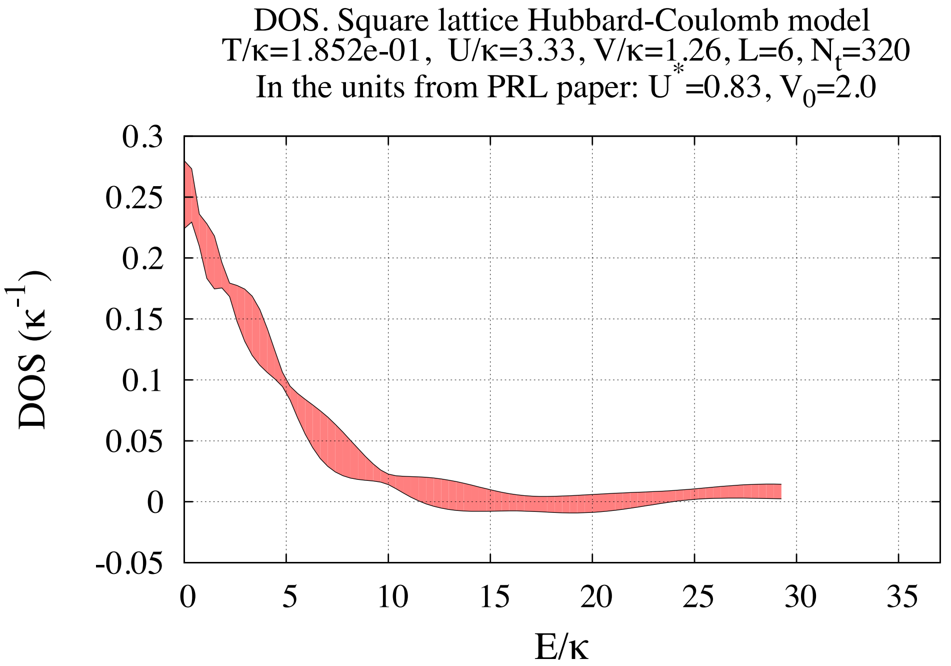


T. Stauber et al., arXiv:1704.03747, to appear in PRL

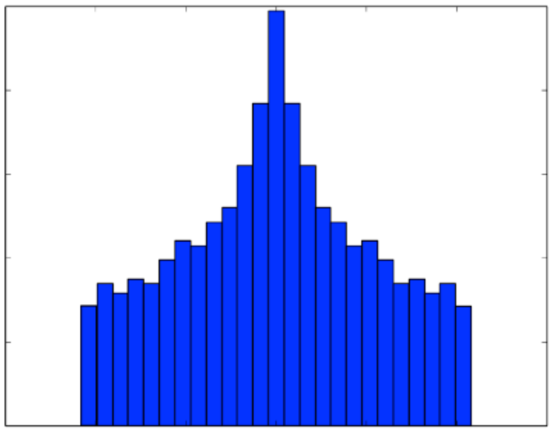
Revealing the artifacts in QMC data

Important, that we can reveal the artifacts in our Monte Carlo data which appear due to the discretization errors:



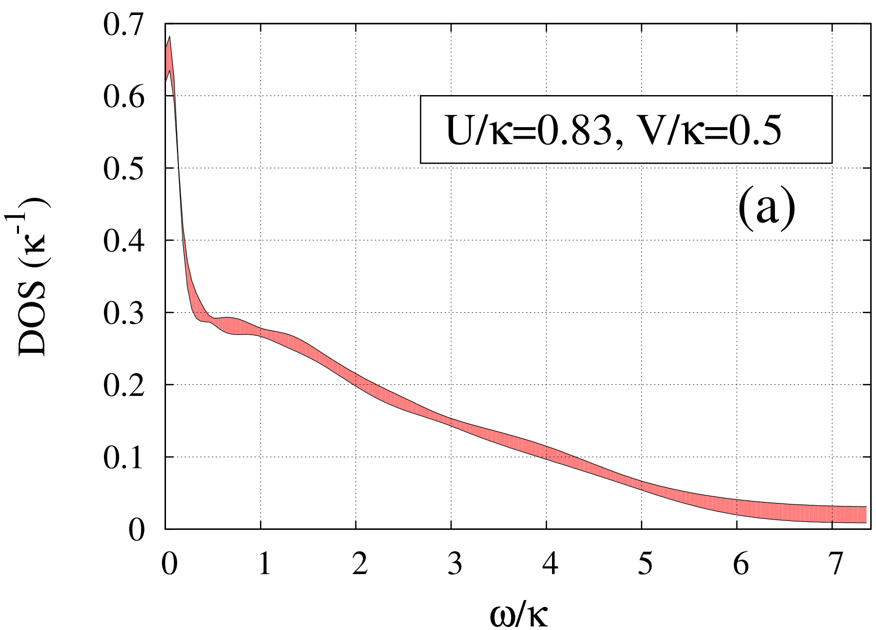


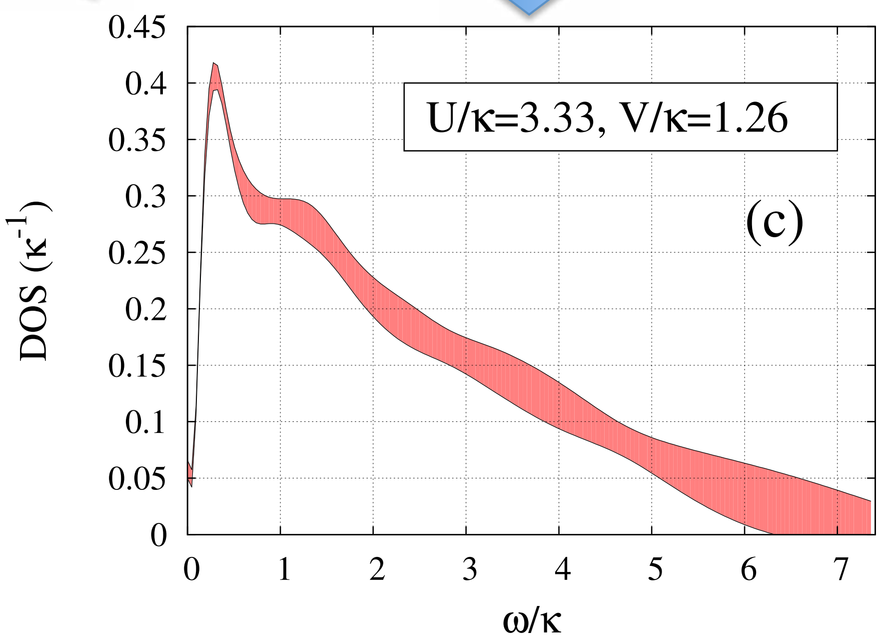
Phase transition in Hubbard-Coulomb model on square lattice (1)



Free fermions

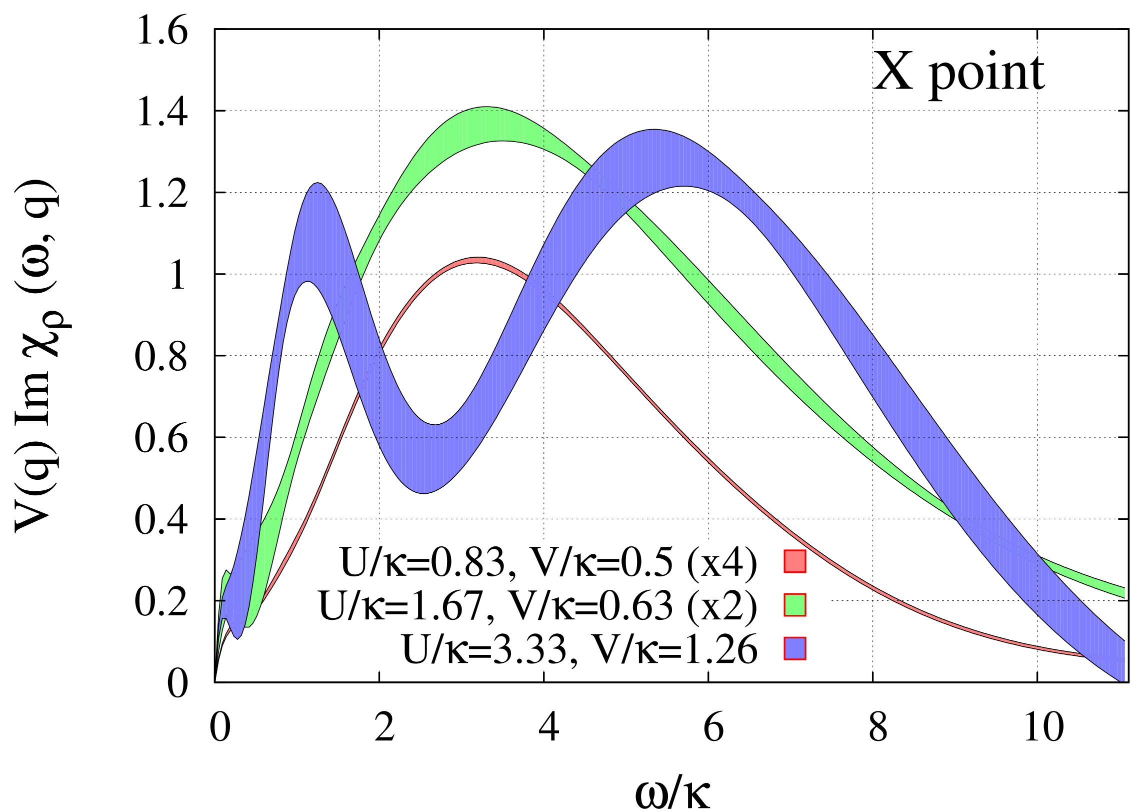
Interacting fermions





Phase transition in Hubbard-Coulomb model on square lattice (2)

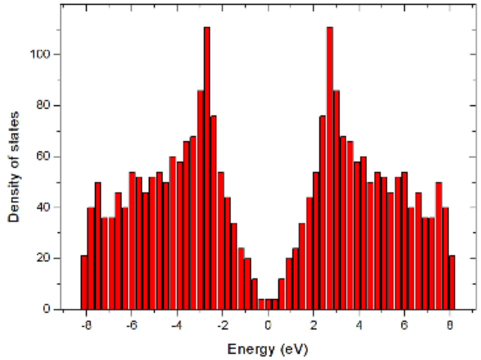
Splitting of dispersion relation of plasmons from momentum-resolved charge susceptibility:



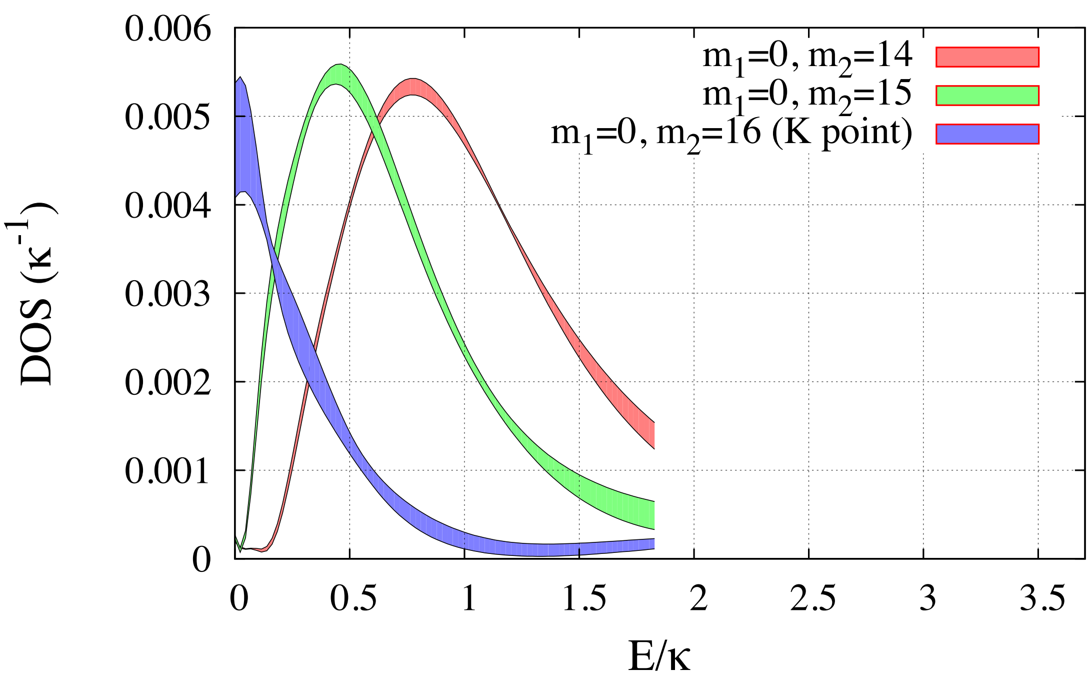
to appear in ArXiv

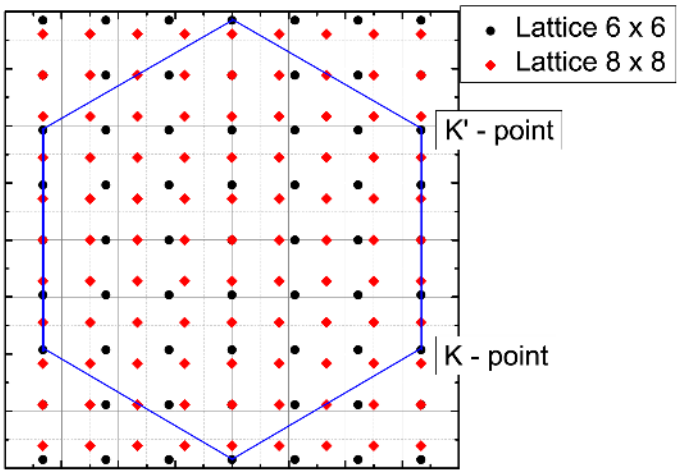
Phase transition in Hubbard model on hexagonal lattice (1)

In the case of semi-metal, we need to use momentum-resolved DOS.

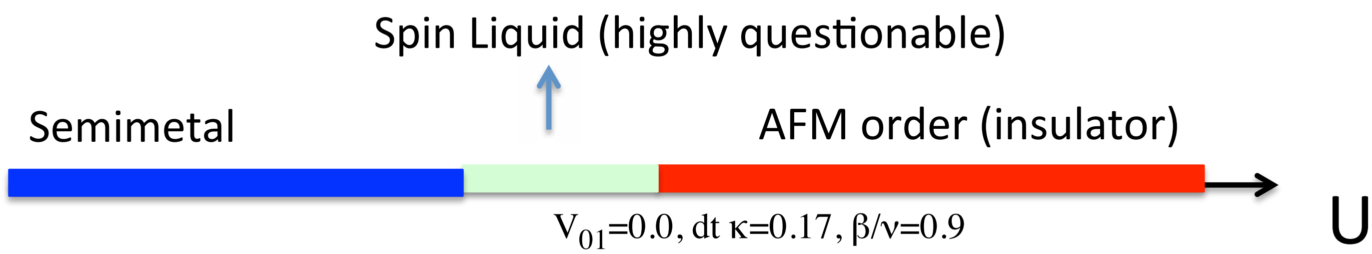


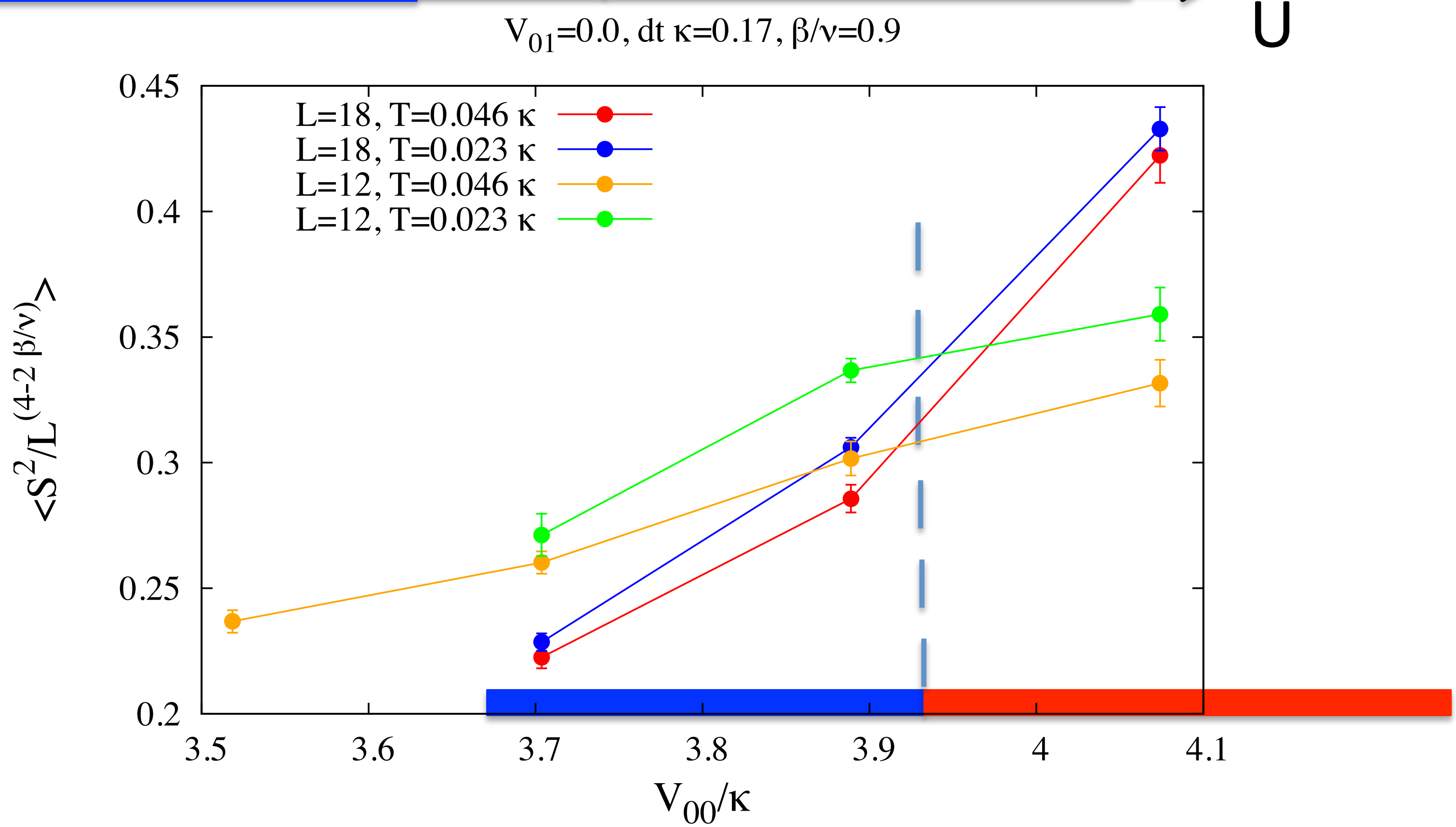
DOS. T/κ=2.315e-02, suspended graphene, L=24, N_t=160



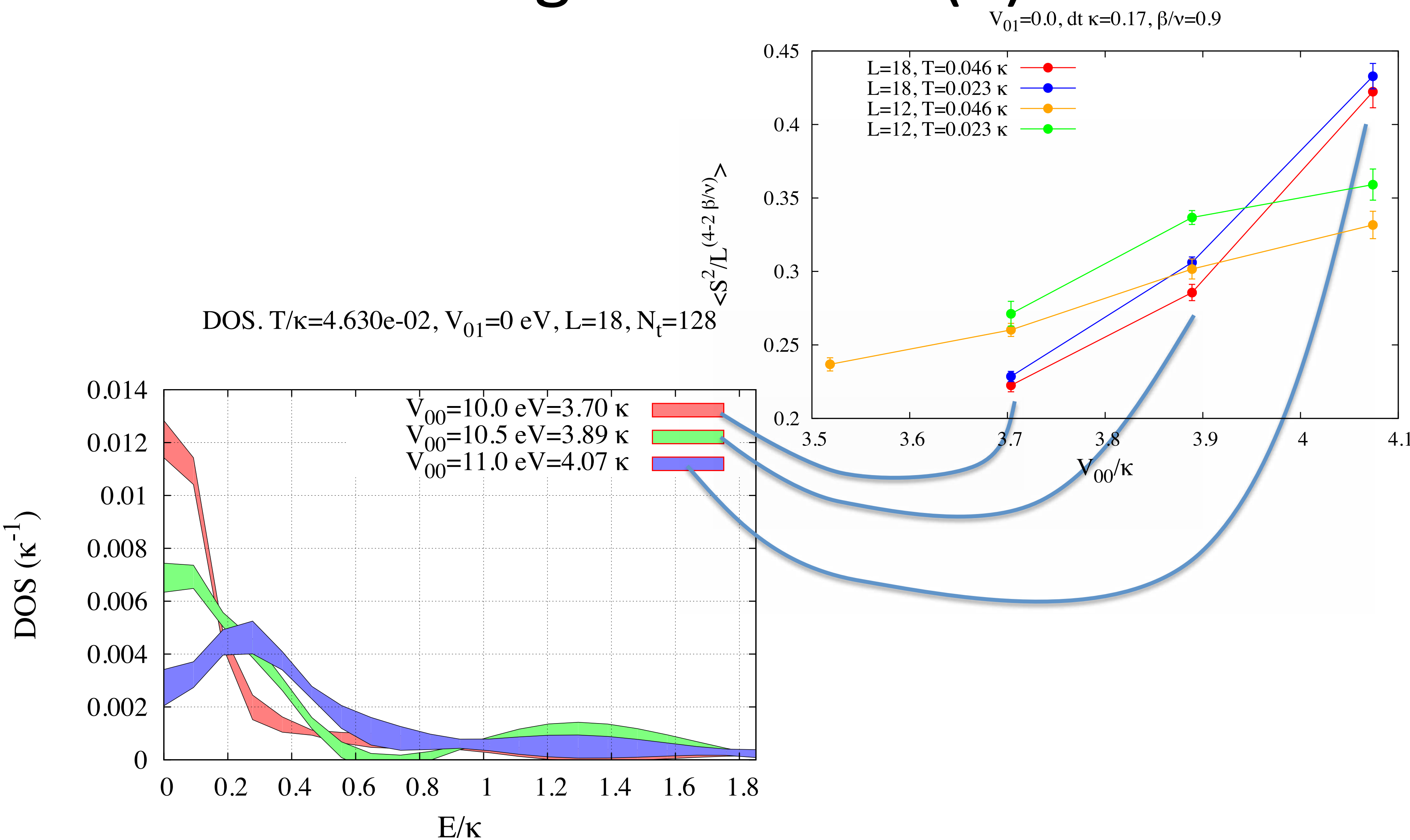


Phase transition in Hubbard model on hexagonal lattice (2)

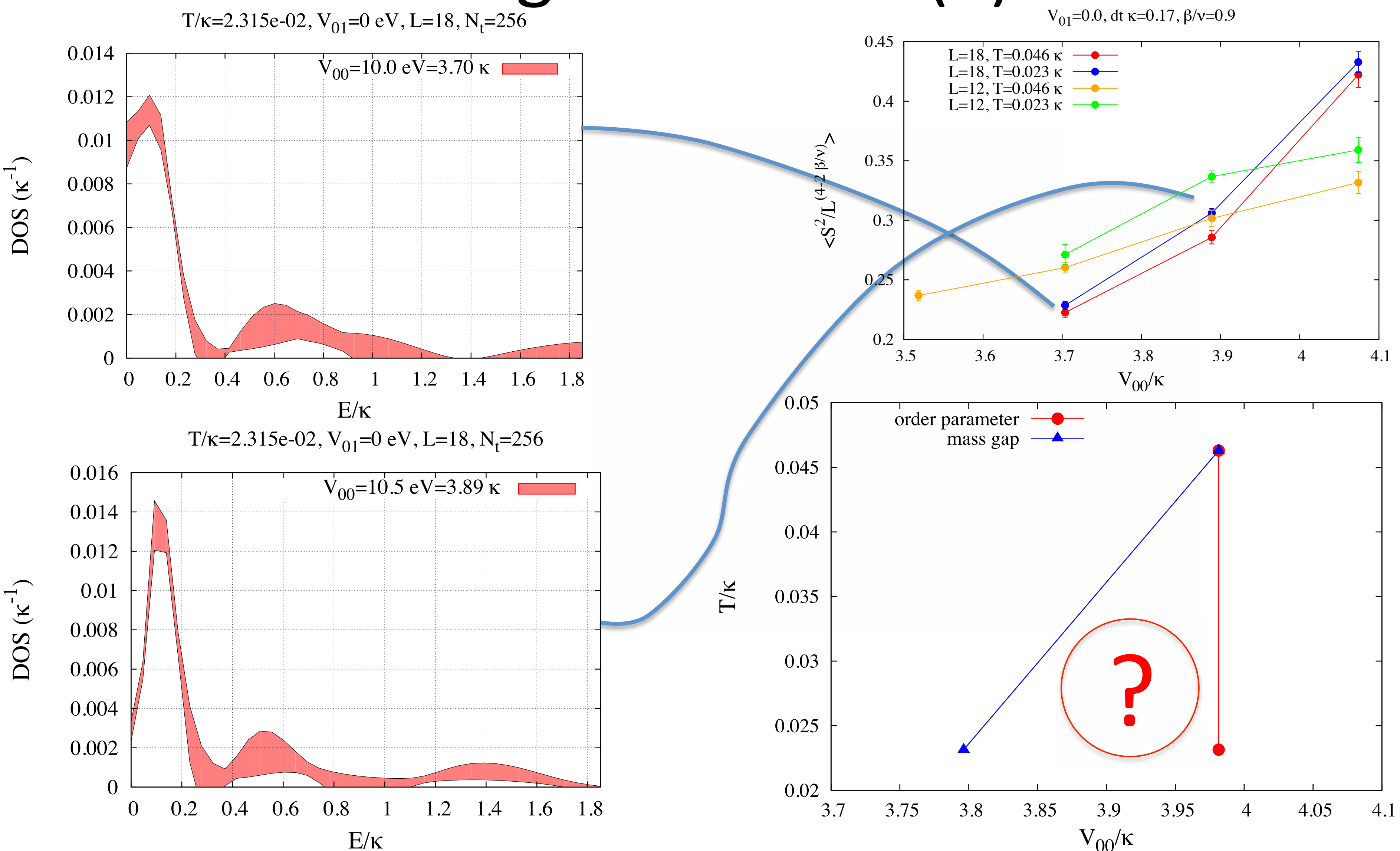




Phase transition in Hubbard model on hexagonal lattice (3)



Phase transition in Hubbard model on hexagonal lattice (4)



Summary

- Unbiased and efficient methods for analytical continuation are highly desirable in the situations, where neither the nature nor the position of the phase transition is known.
- Proposed modifications of the BG method lead to sufficient increase of it’s resolution in frequency without sacrificing the stability.
- Applications show that the modified BG method can be useful in the direct detection of the phase transition to the insulating states. We were able to calculate the full and momentum-resolved DOS and locate the position of the phase transition.

Code can be downloaded from GitHub:
https://github.com/ulybyshev/Green-Kubo_solver