Heterostructure project

July 3, 2024

The following plots show NCA results for a heterostructure consisting of two materials: U_1 and U_2 are the corresponding Coulomb interactions.

1 $U_1 = 1.0$ and $U_2 = 10.0$ for 4 sites

K-propagators and populations

In this case we are calculating a heterostructure, where the two materials have different coulomb interactions - one is a correlated metal and the other one is a Mott insulator. The K-propagators seem to be well converged and so do the populations.

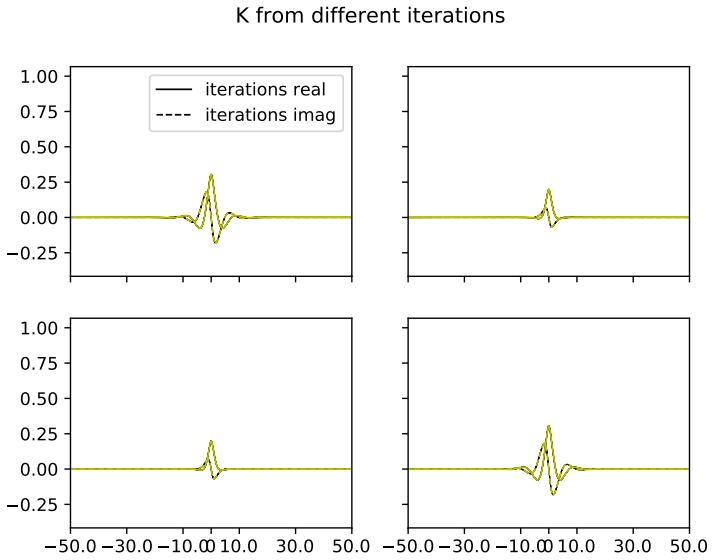

Figure 1: K-propagators for site = 0 and iteration 30.

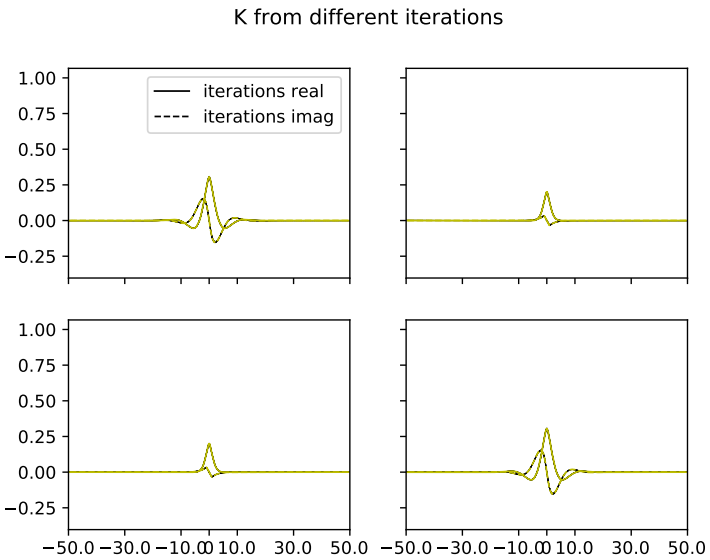

Figure 2: K-propagators for site = 1 and iteration 30.

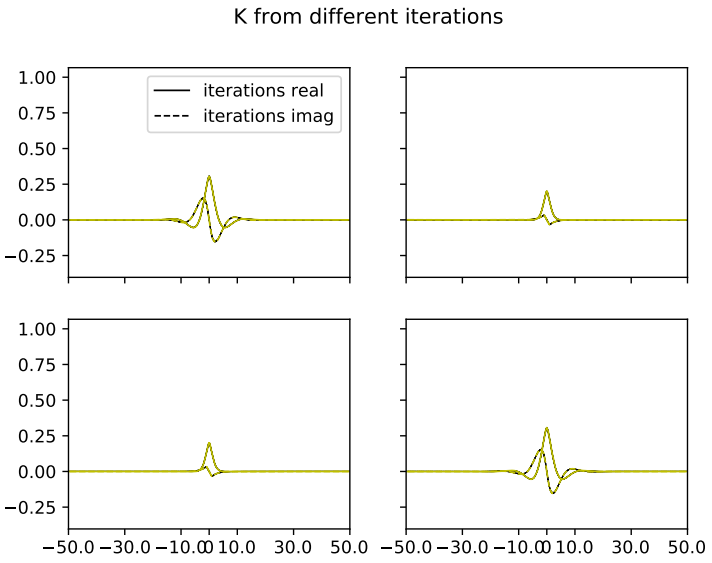

Figure 3: K-propagators for site = 2 and iteration 30.

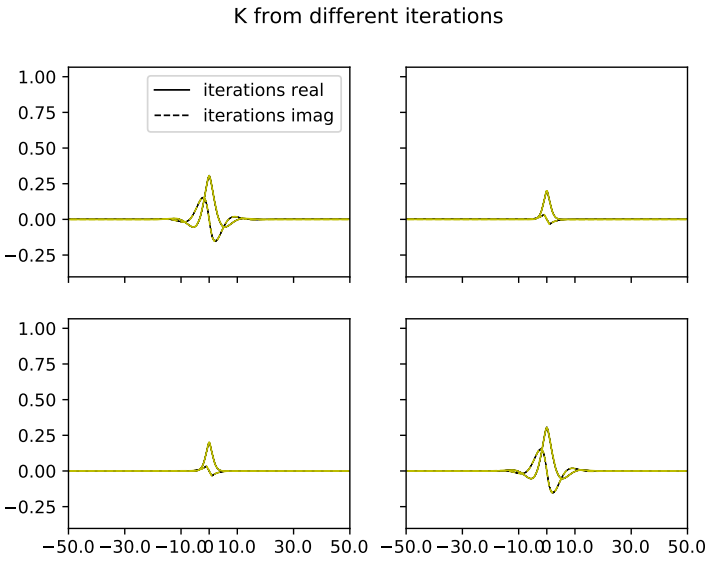

Figure 4: K-propagators for site = 3 and iteration 30.

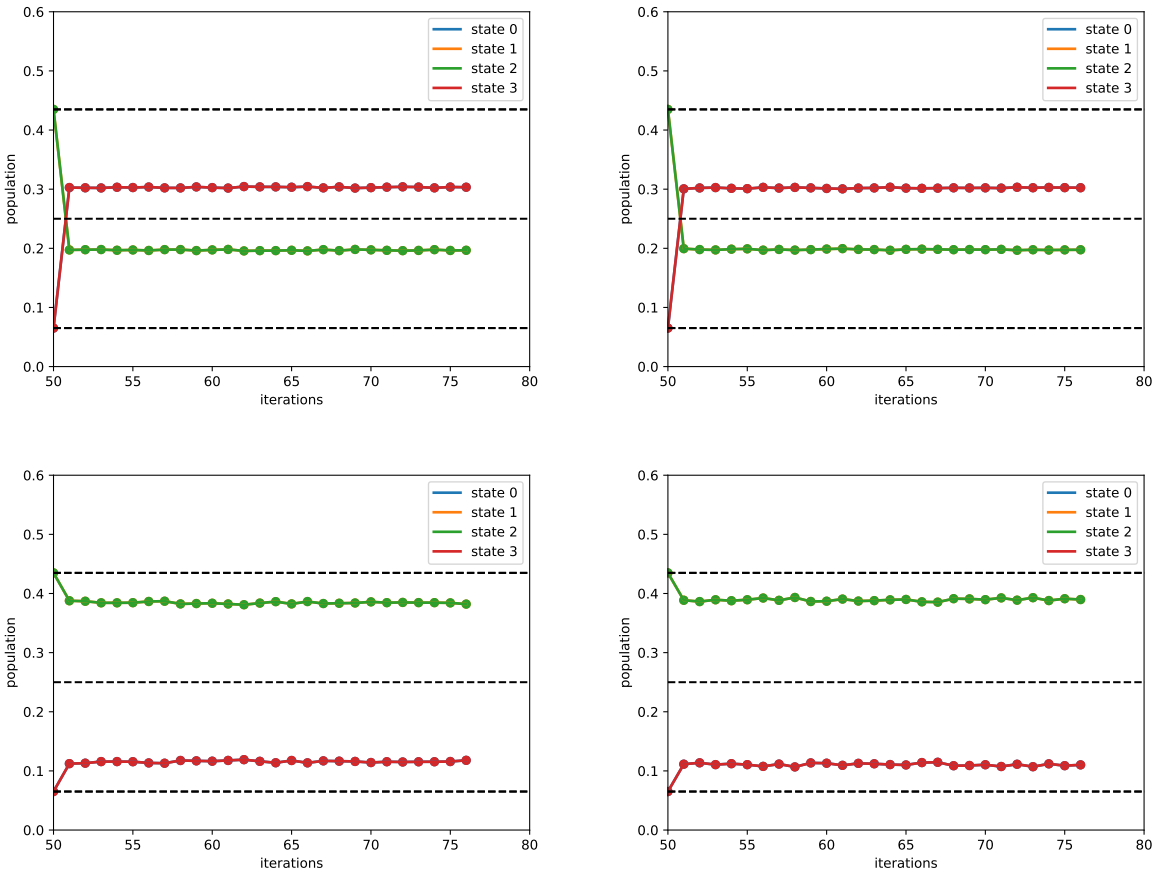

Figure 5: Populations for site = 1 (upper left) and site = 2 (upper right) and site = 3 (lower left) and site = 4 (lower right) for iteration 30.

Greens functions

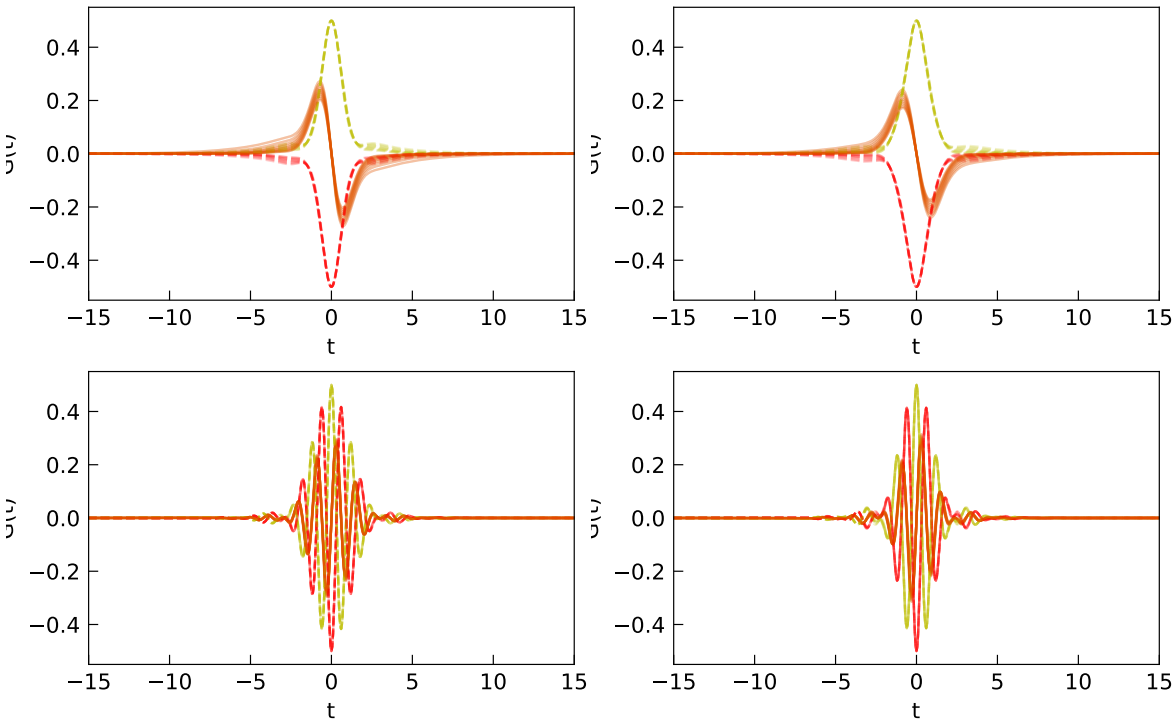

Figure 6: $G^<$ yellow, $G^>$red, solid lines are real part and dotted imaginary; site = 1 (upper left) and site = 2 (upper right) and site = 3 (lower left) and site = 4 (lower right) for iteration 10 until 30.

Spectral functions

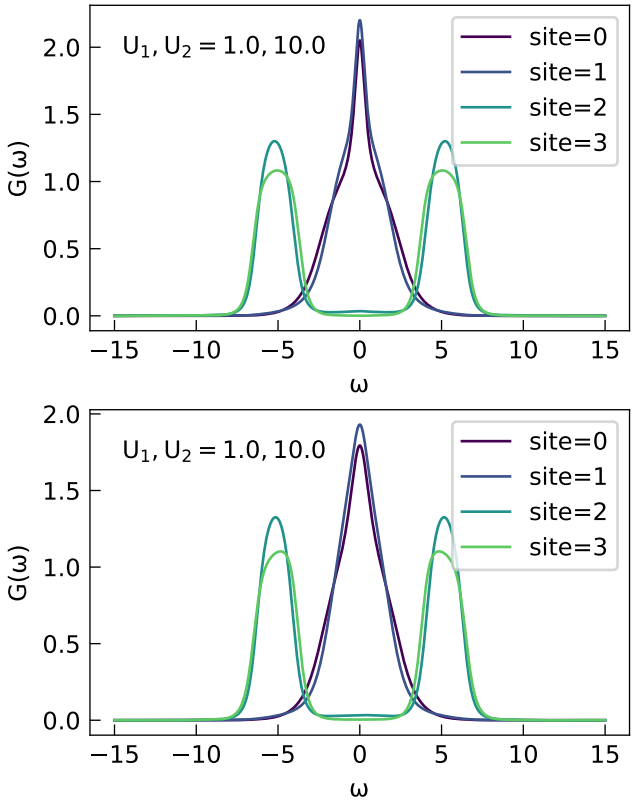

Figure 7: Spectral function for all sites at iteration 10 and 20.

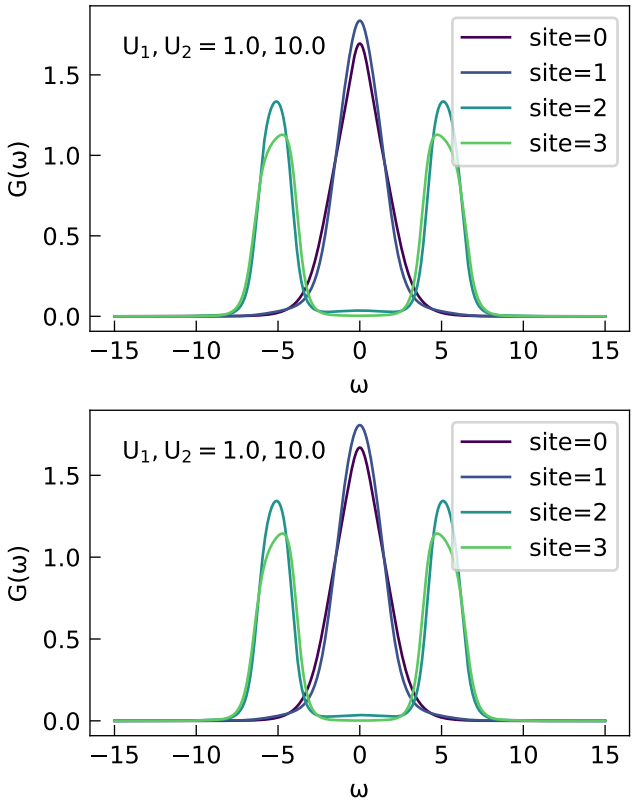

Figure 8: Spectral function for all sites at iteration 30 and 35.

2 $U_1 = 1.0$ and $U_2 = 6.0$ for 8 sites

K-propagators and populations

site 0

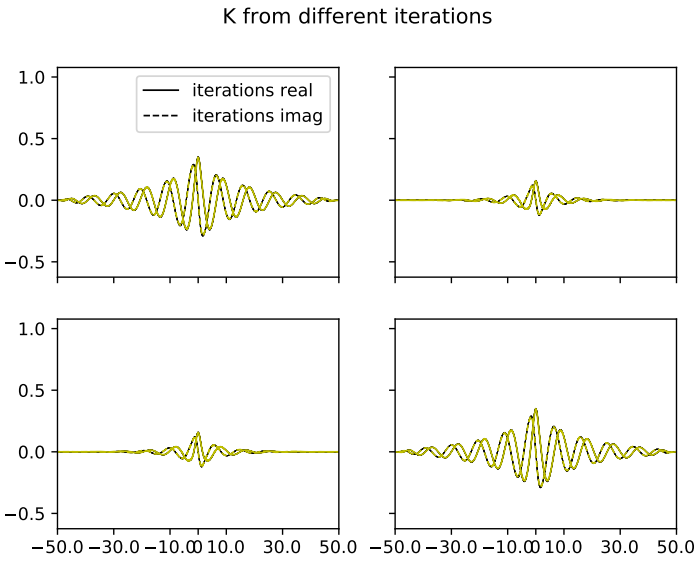

Figure 9: K-propagators for site = 0 and iteration 0.

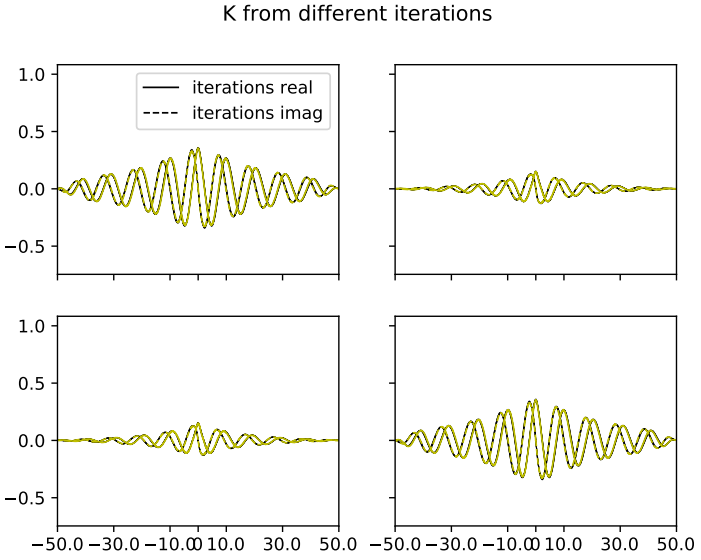

Figure 10: K-propagators for site = 0 and iteration 4.

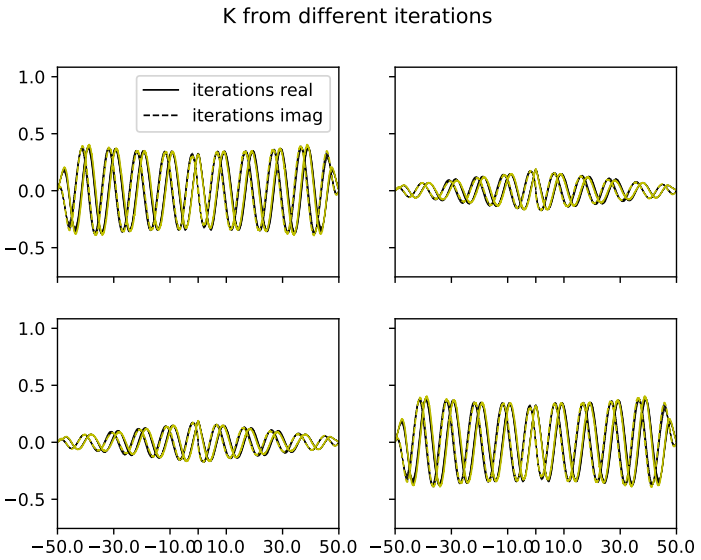

Figure 11: K-propagators for site = 2 and iteration 5.

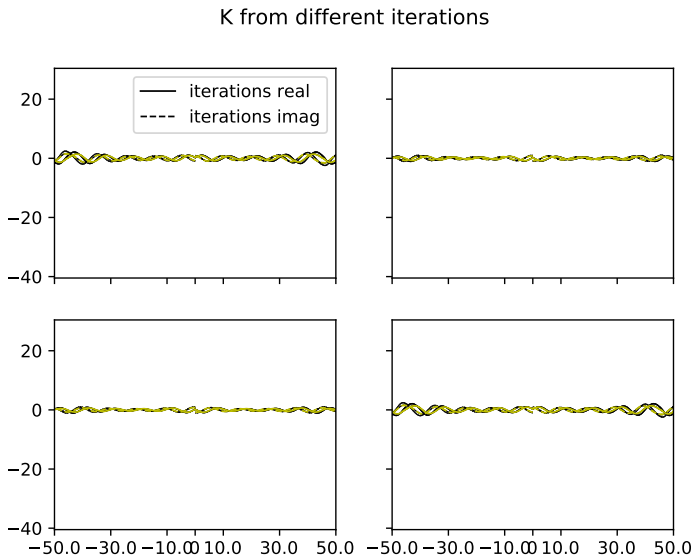

Figure 12: K-propagators for site = 3 and iteration 6.

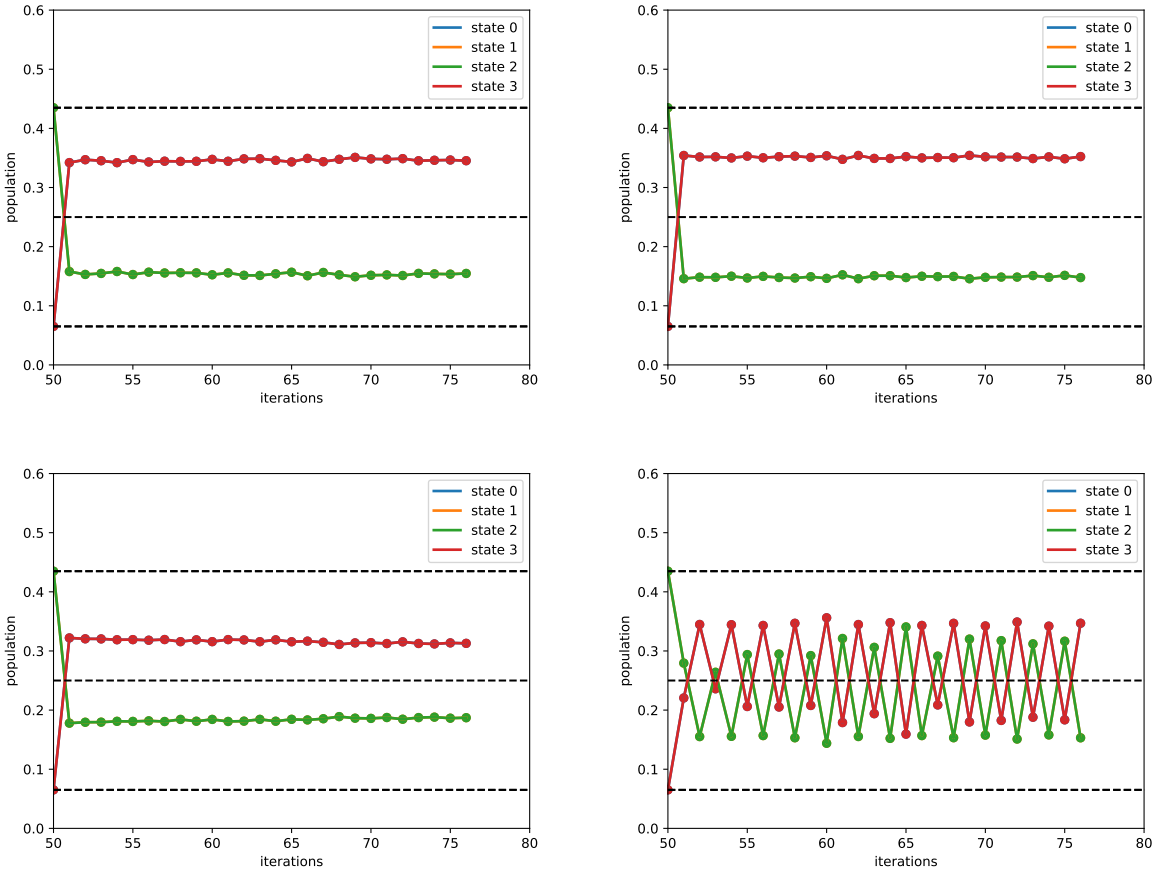

Figure 13: Populations for iteration=0 (upper left), iteration=4 (upper right), iteration=5 (lower left) and iteration=6 (lower right).

Greens functions

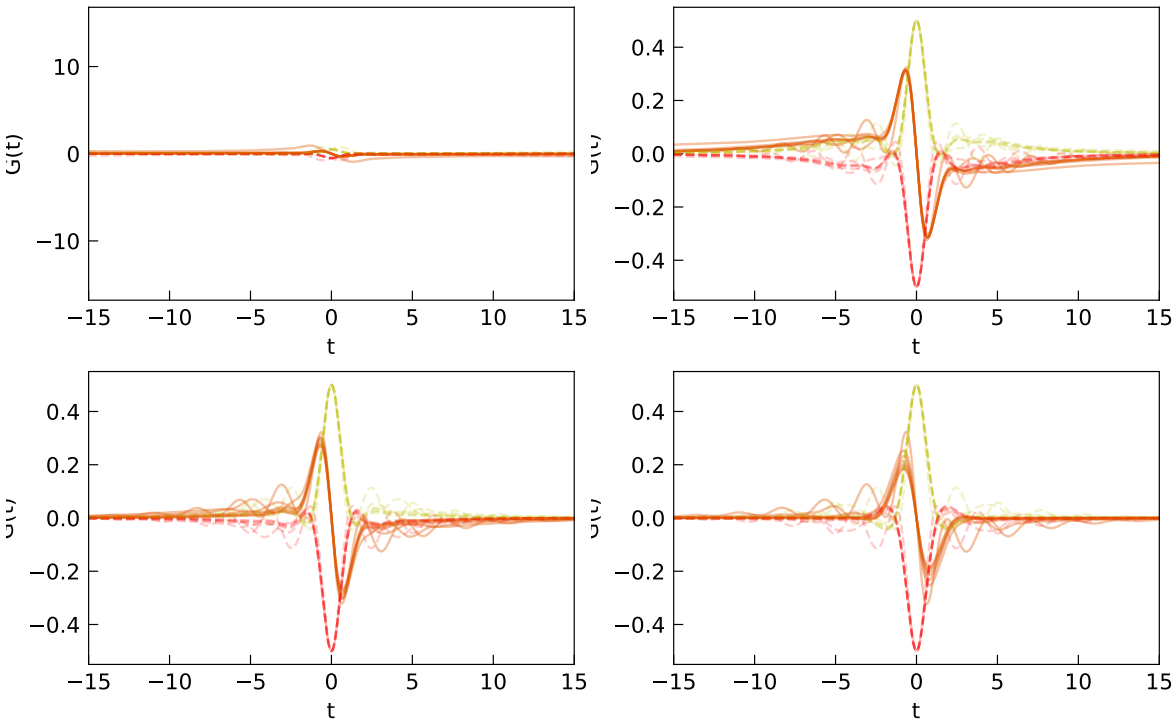

Figure 14: $G^<$ yellow, $G^>$red, solid lines are real part and dotted imaginary; site = 1 (upper left) and site = 2 (upper right) and site = 3 (lower left) and site = 4 (lower right) for iteration 0 until 6.

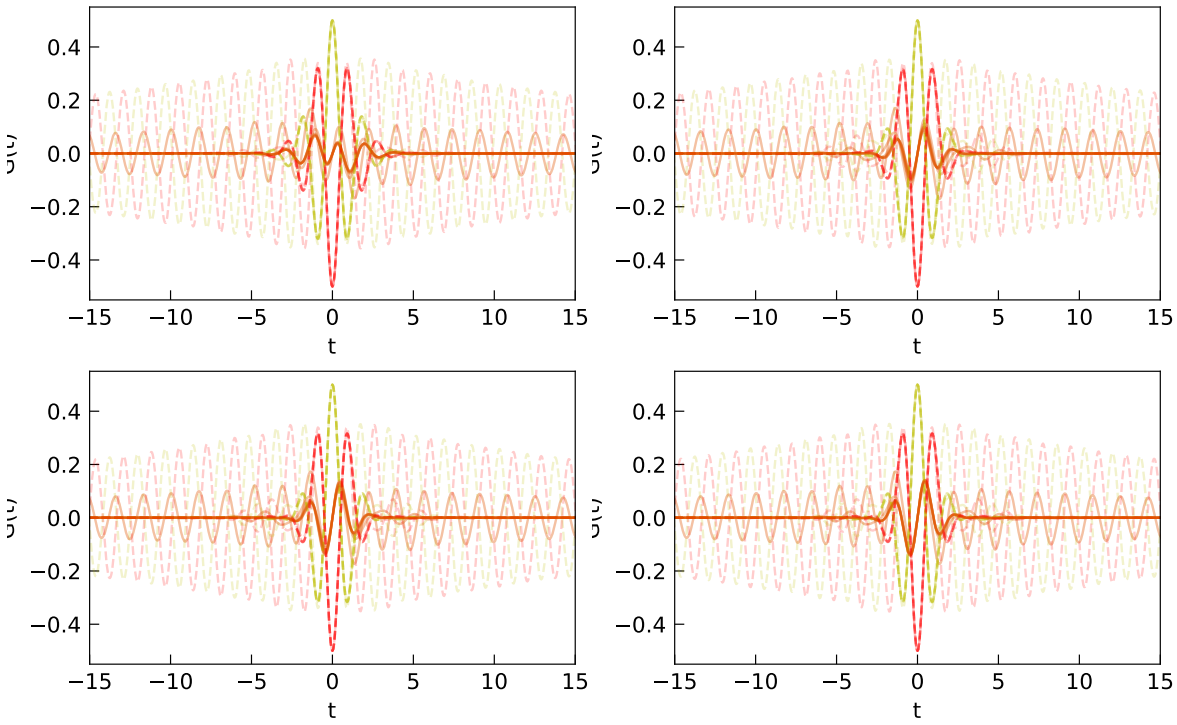

Figure 15: $G^<$ yellow, $G^>$red, solid lines are real part and dotted imaginary; site = 5 (upper left) and site = 6 (upper right) and site = 7 (lower left) and site = 8 (lower right) for iteration 0 until 6.

Spectral functions

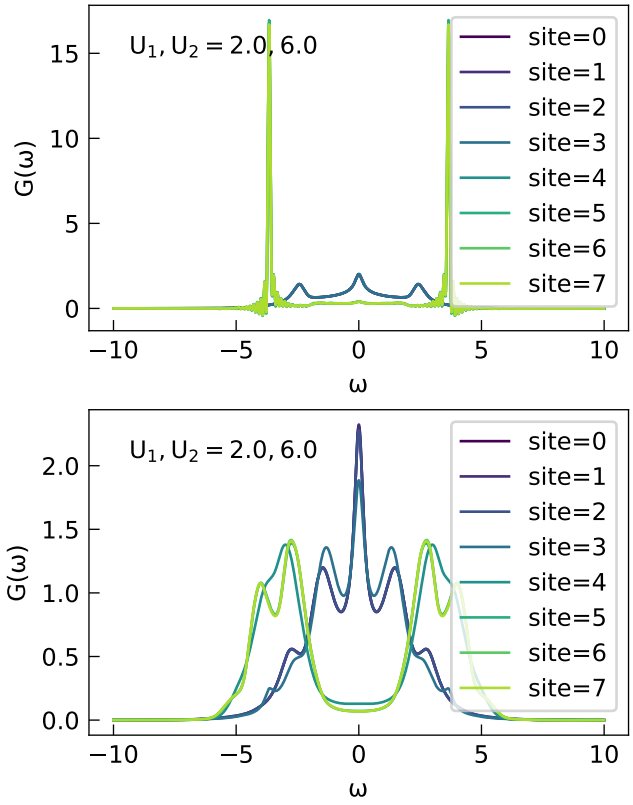

Figure 16: Spectral function for all sites at iteration 0 and 1.

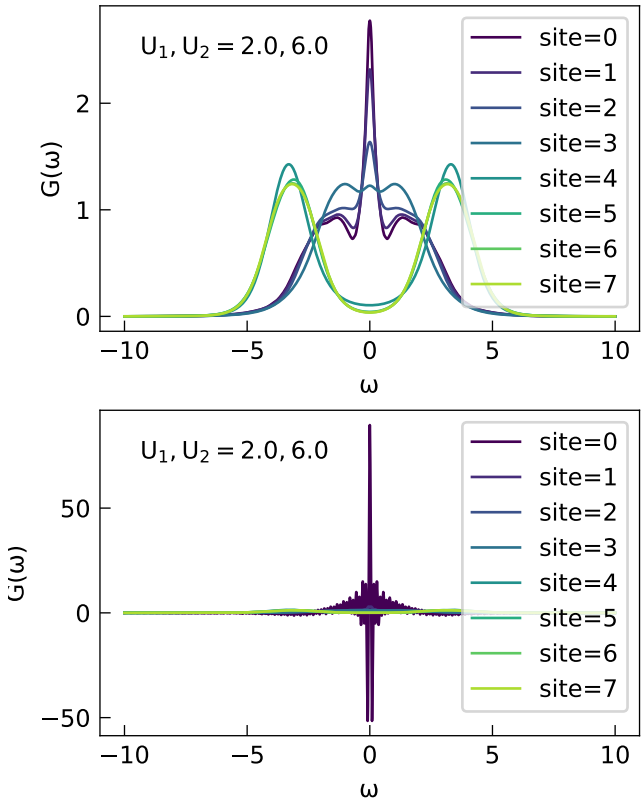

Figure 17: Spectral function for all sites at different iteration 4 and 6.