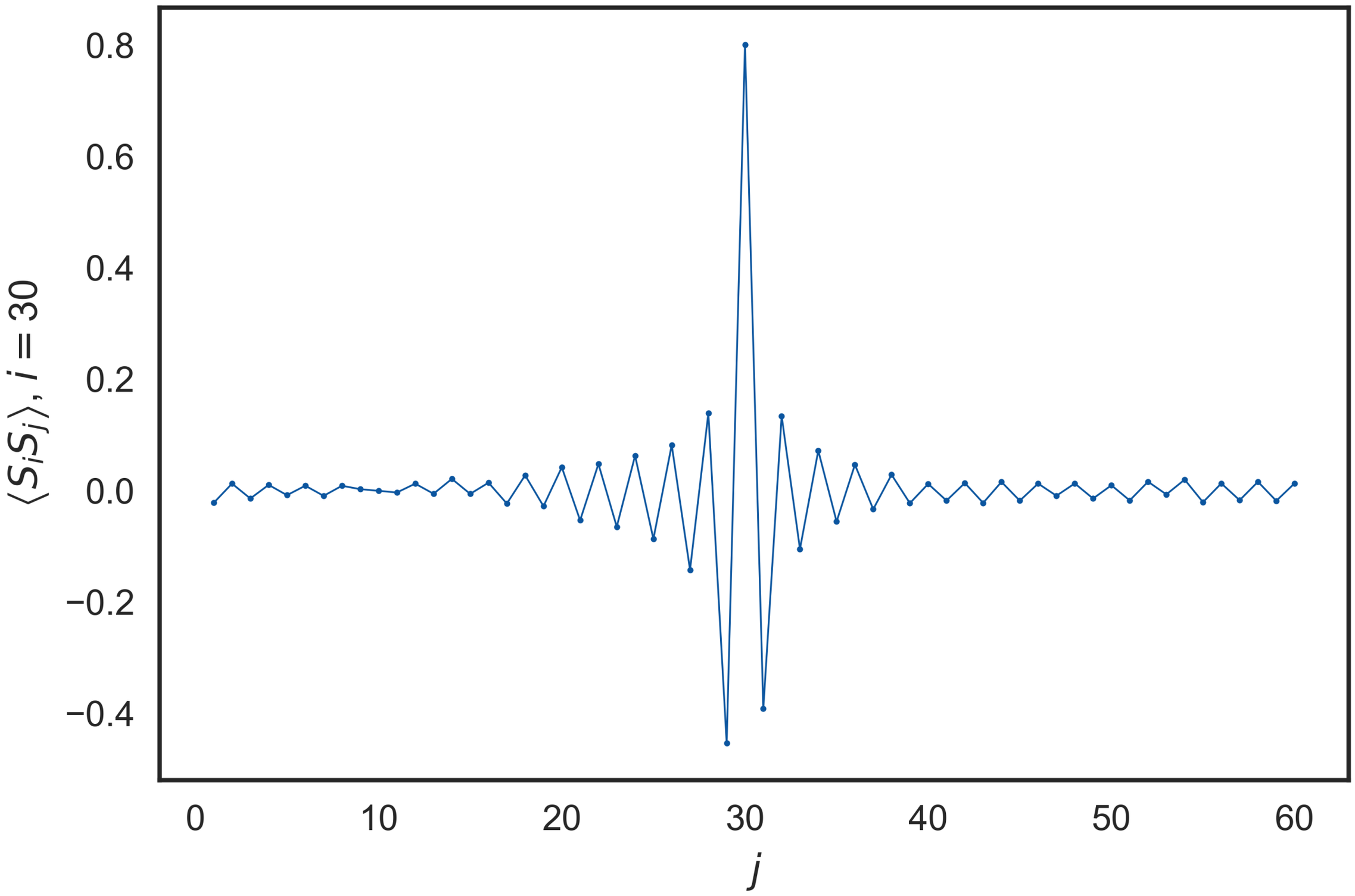
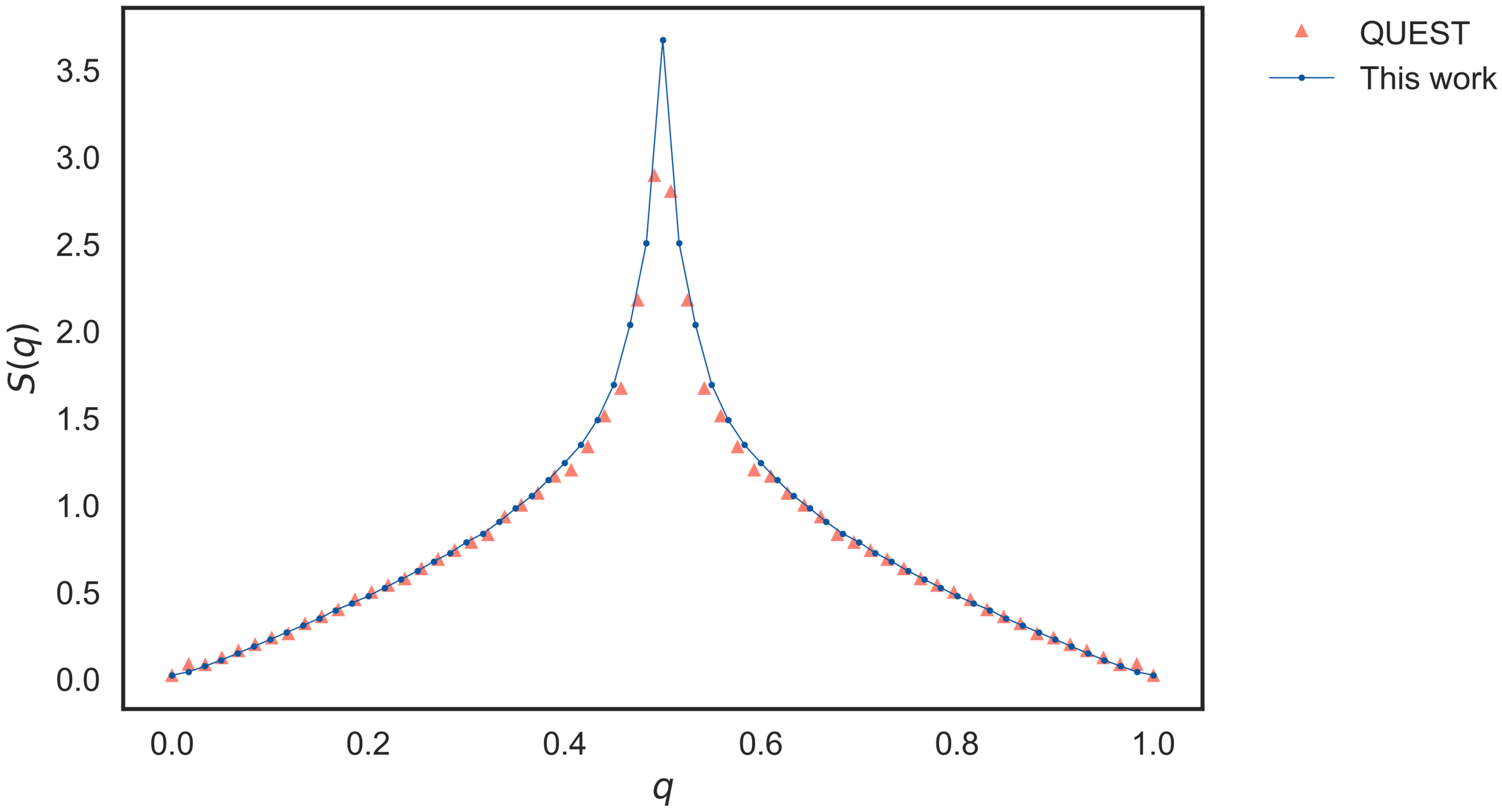
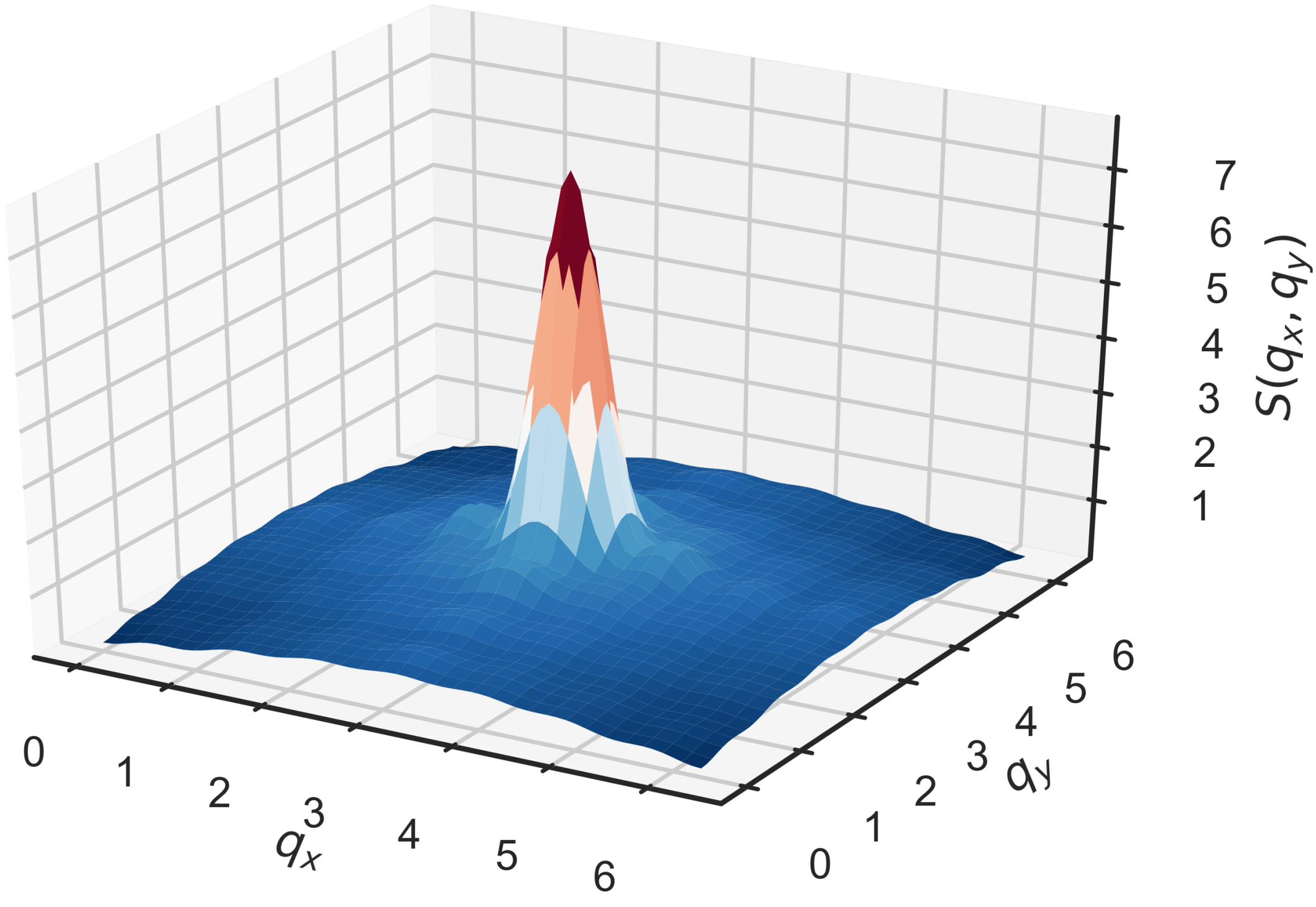
1D, 60 site PBC chain, $\beta = 15$,showing antiferromagnetic ordering



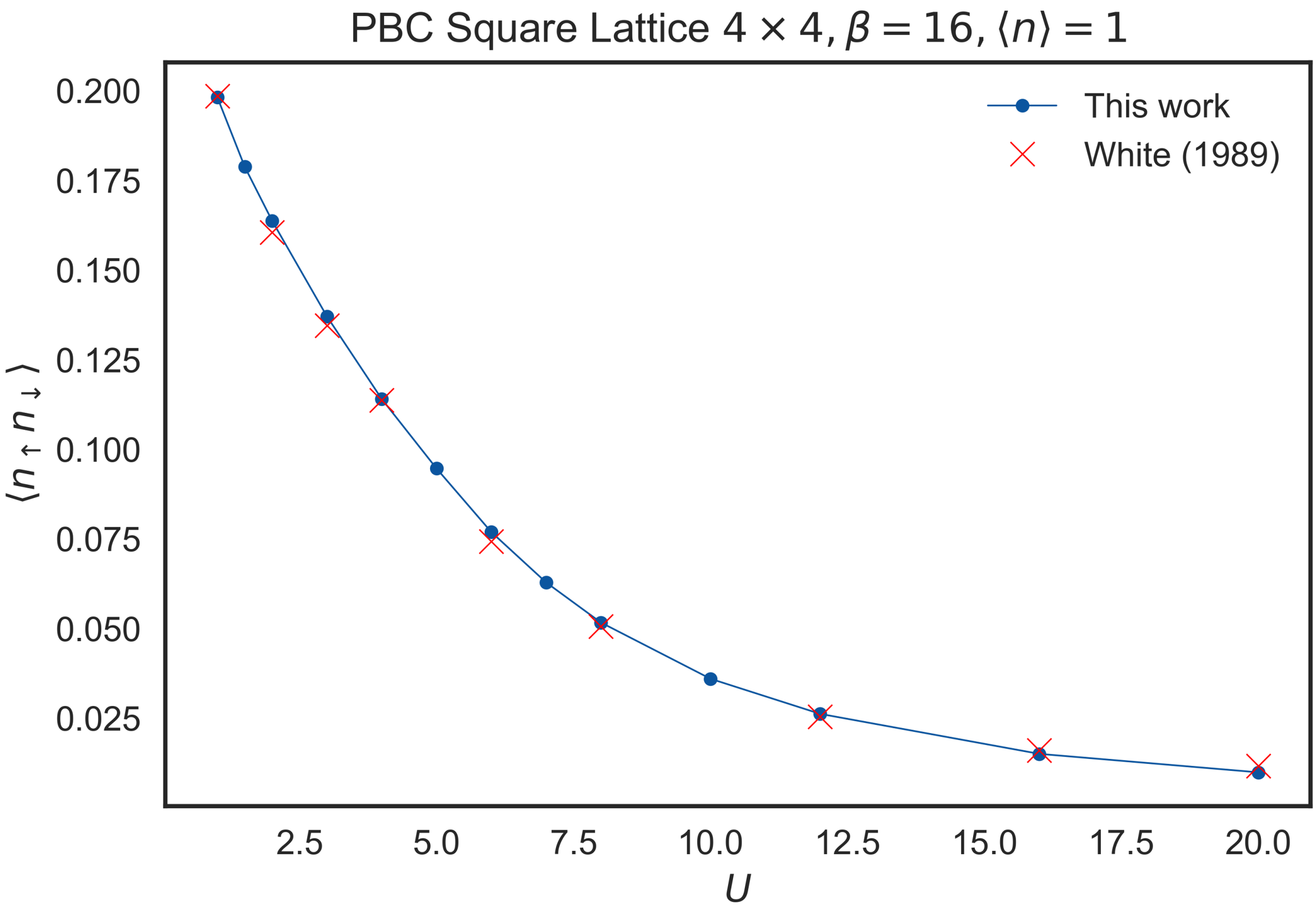
The magnetic structure factor shows a peak at $q = \pi$



A similar reasoning is valid in 2D, for a PBC square lattice with 64 sites at $\beta = 12$

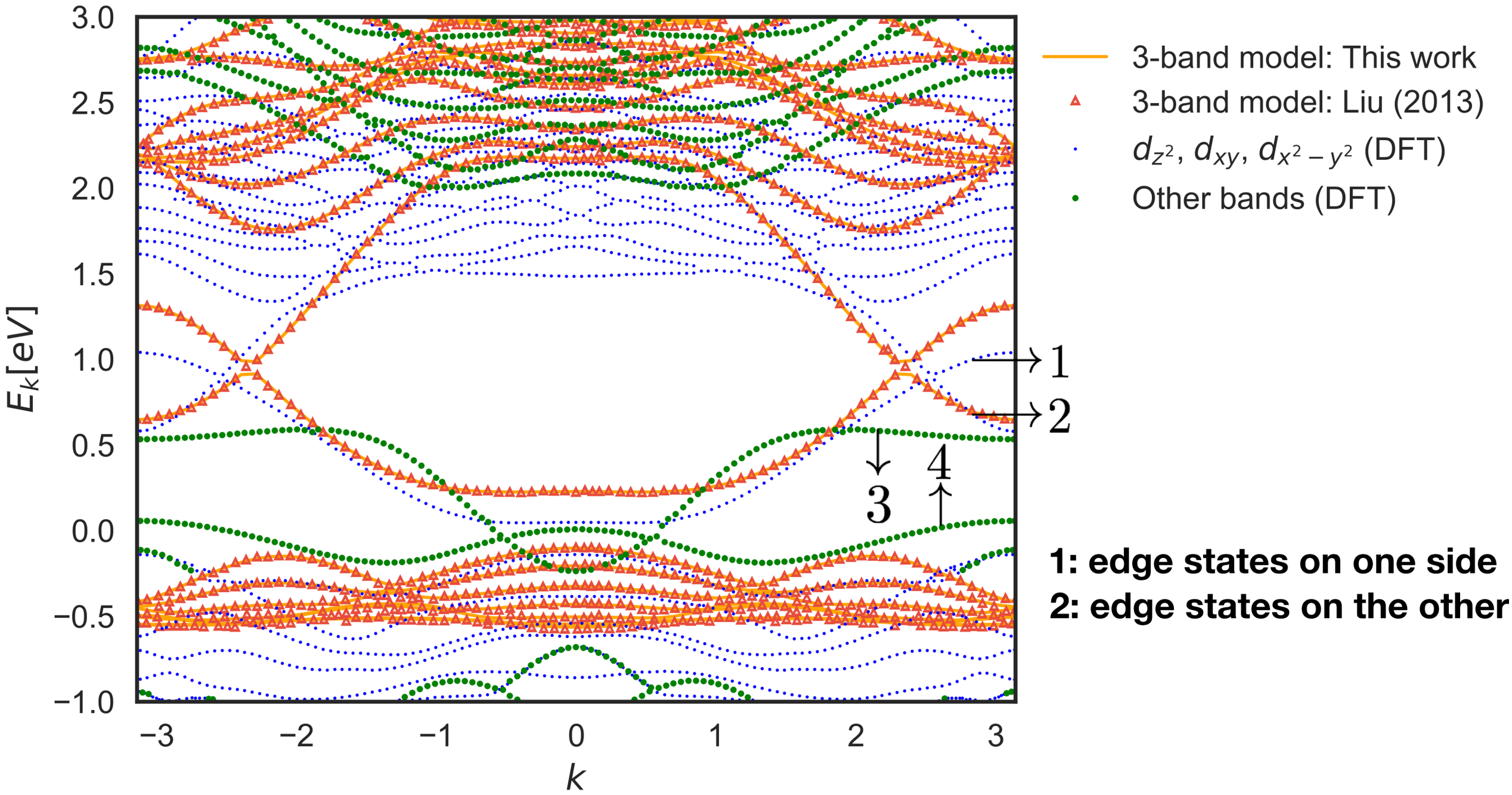


Still on the square lattice, increasing U, the double occupancy decreases



TMDs

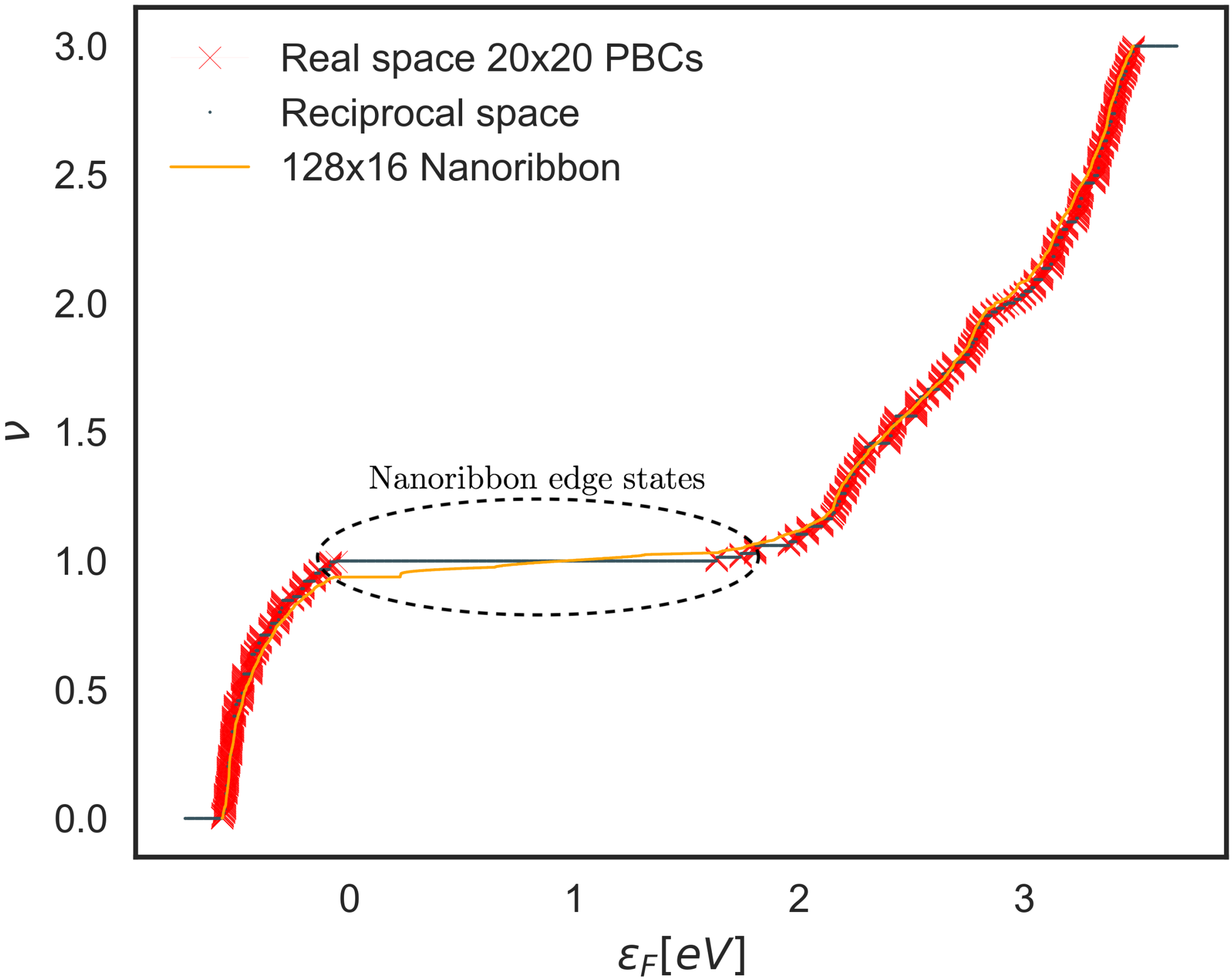
Band structure of a TMD nanoribbon



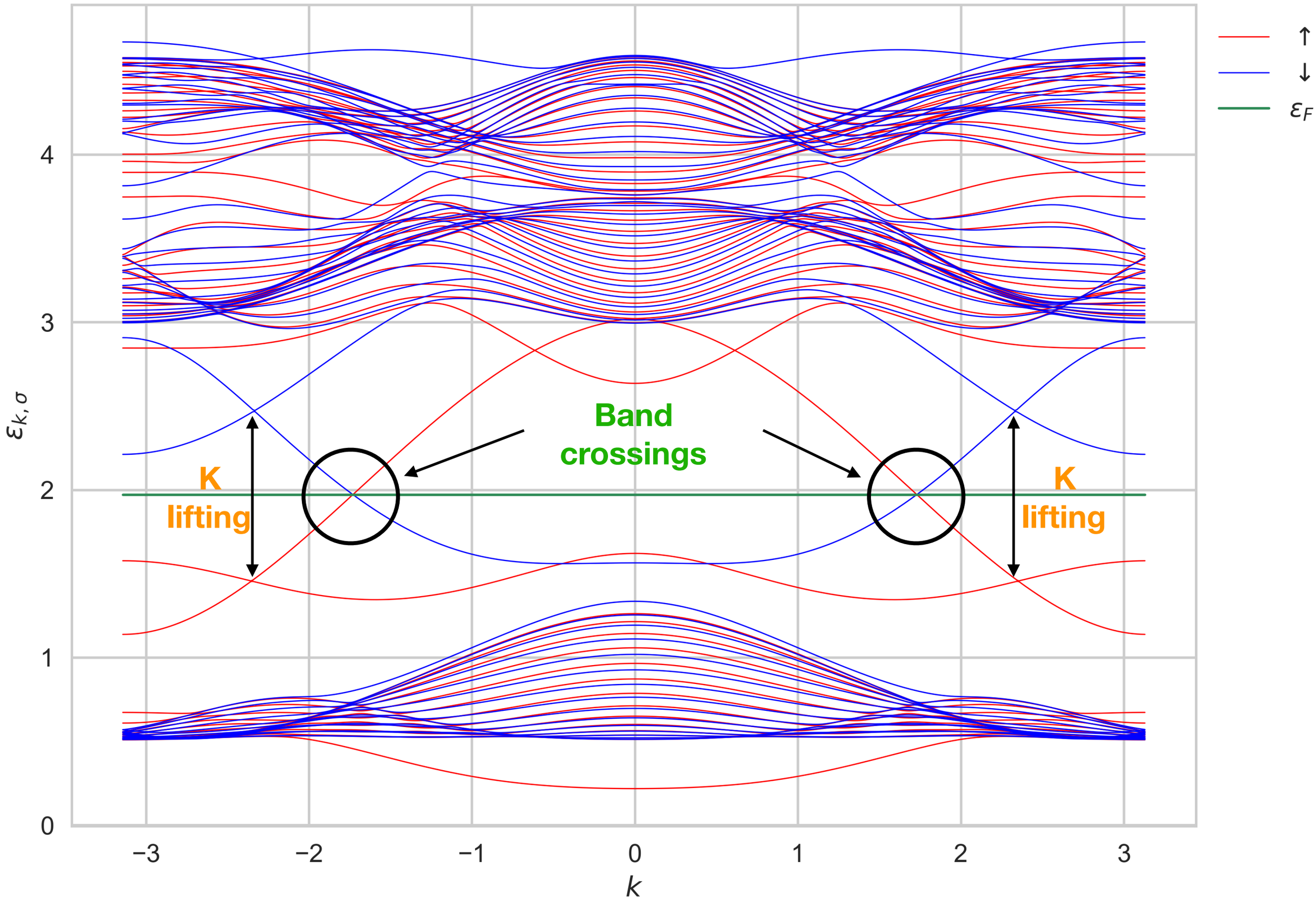
1: edge states on one side

2: edge states on the other

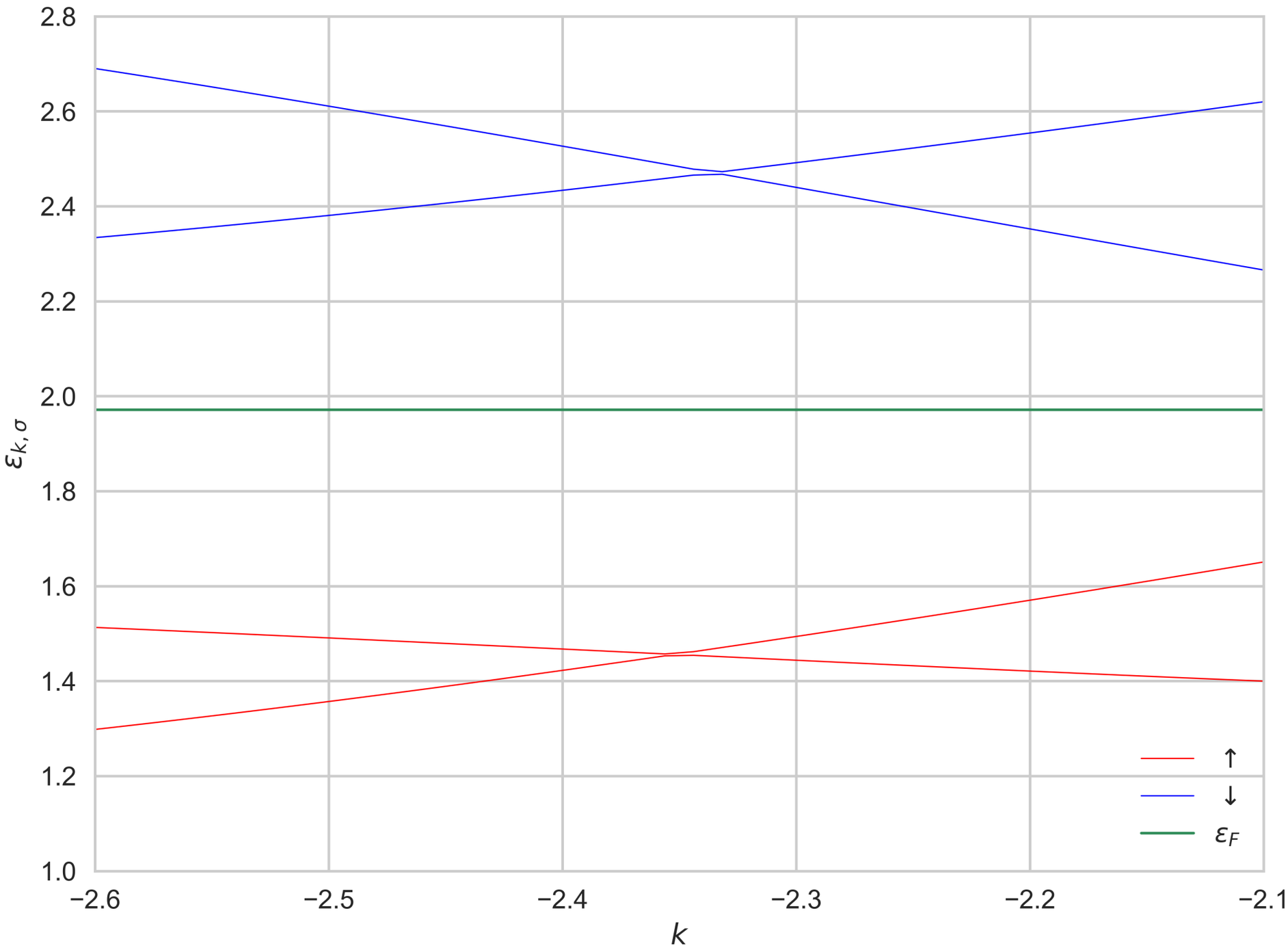
Filling of a TMD monolayer vs nanoribbon



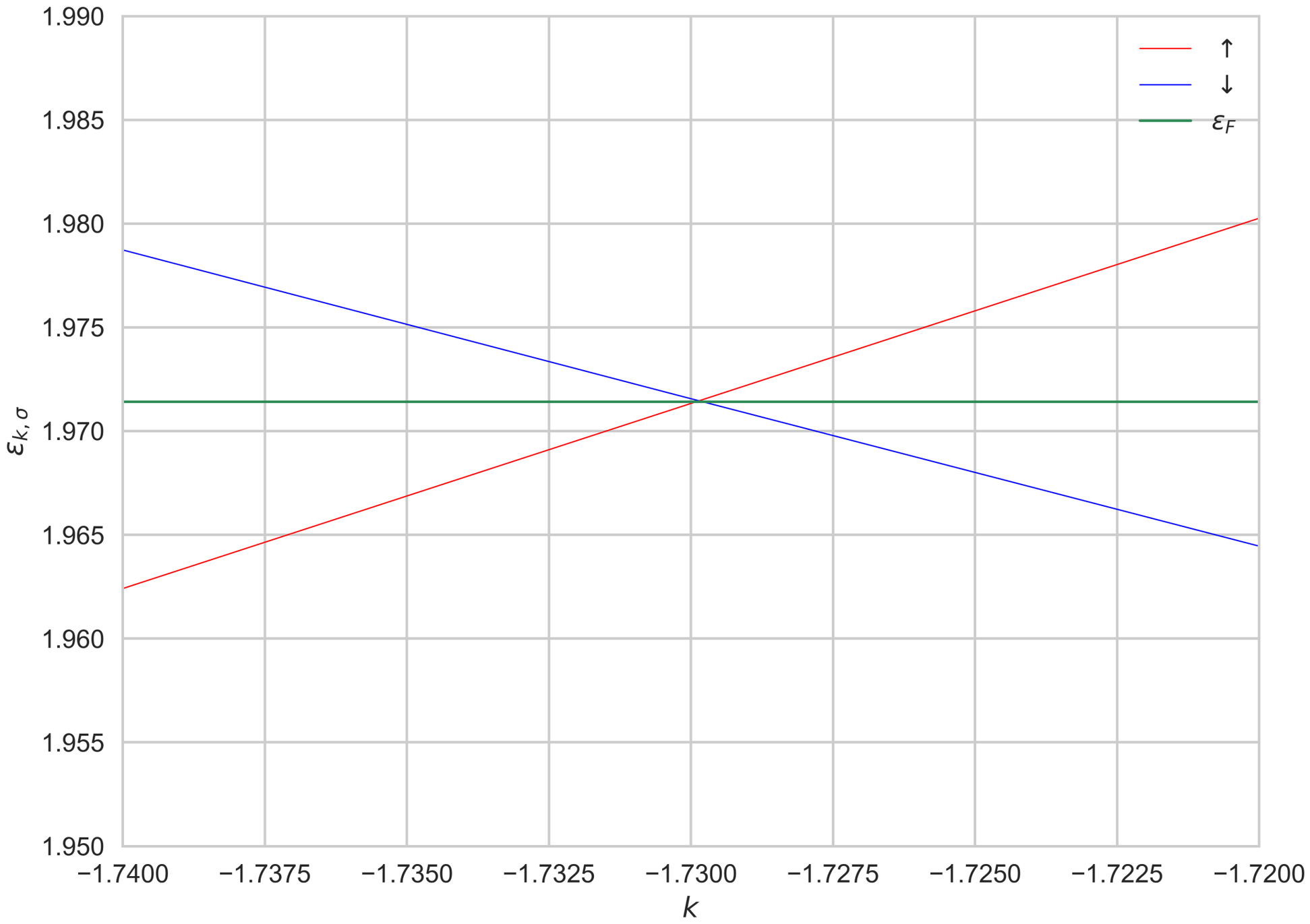
MF band structure for $N_k = 512, N_y = 16, U = 20, T = 0$



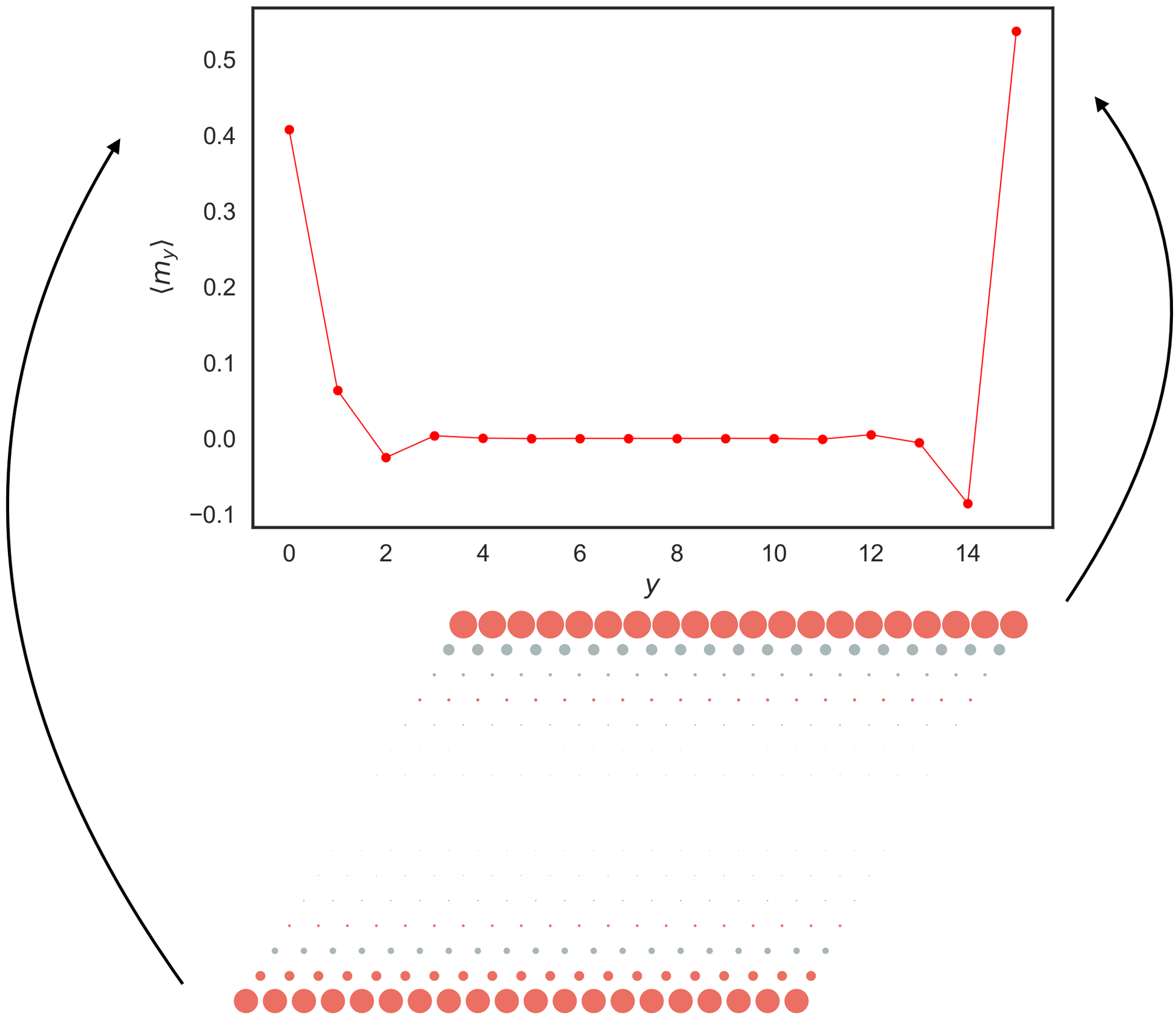
K lifting


2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
$\varepsilon_{k,\sigma}$
−2.6
−2.5
−2.4
−2.3
−2.2
−2.1
k
↑
↓
ε_F

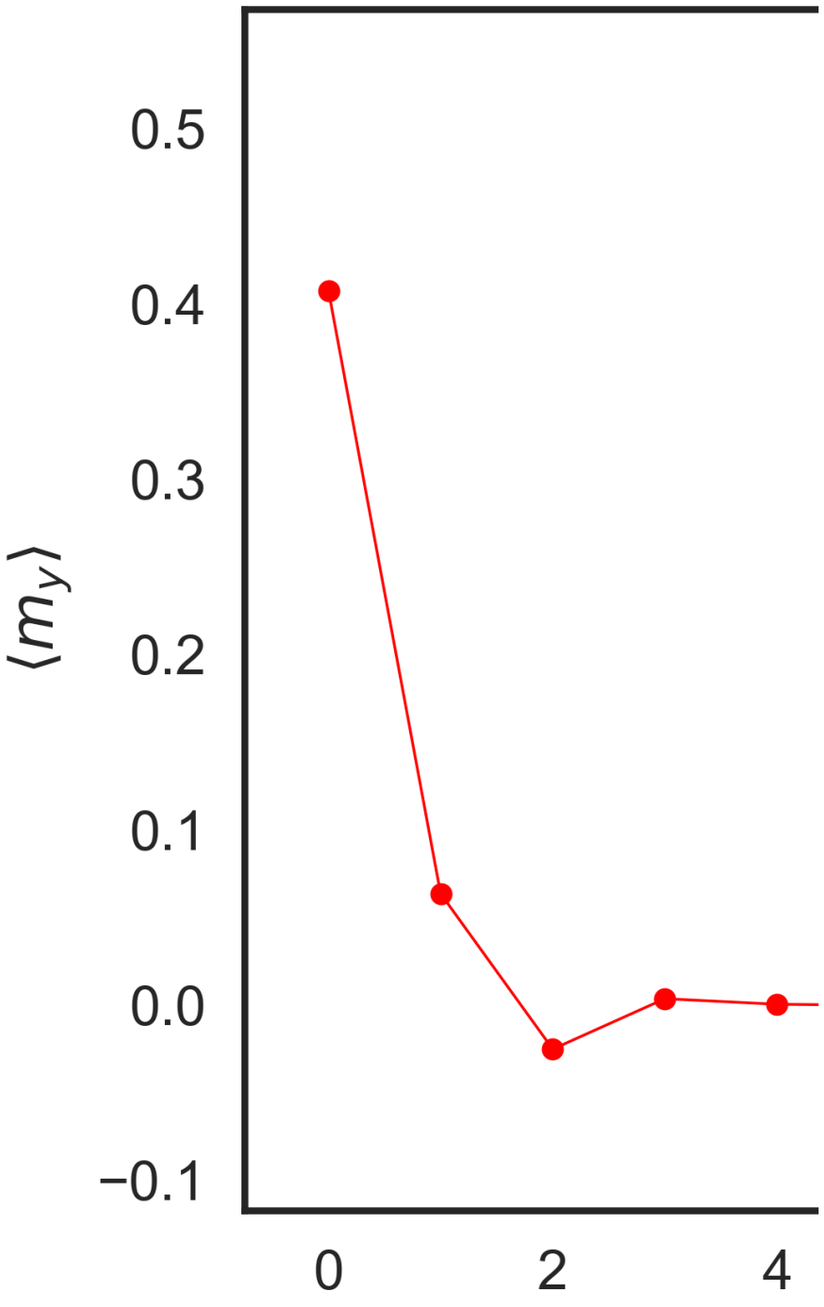
Band crossings

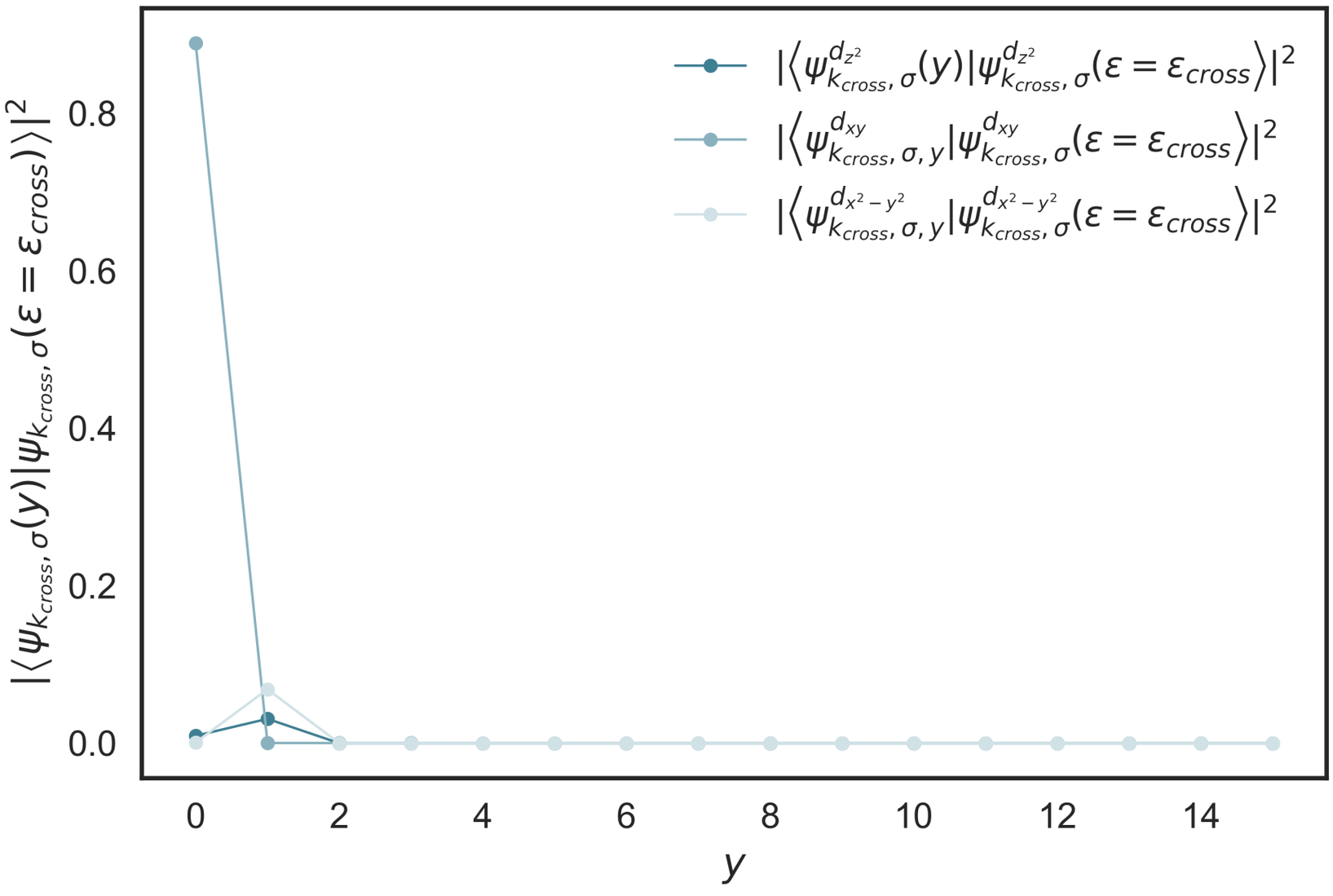


S^z along the transverse direction of the ribbon



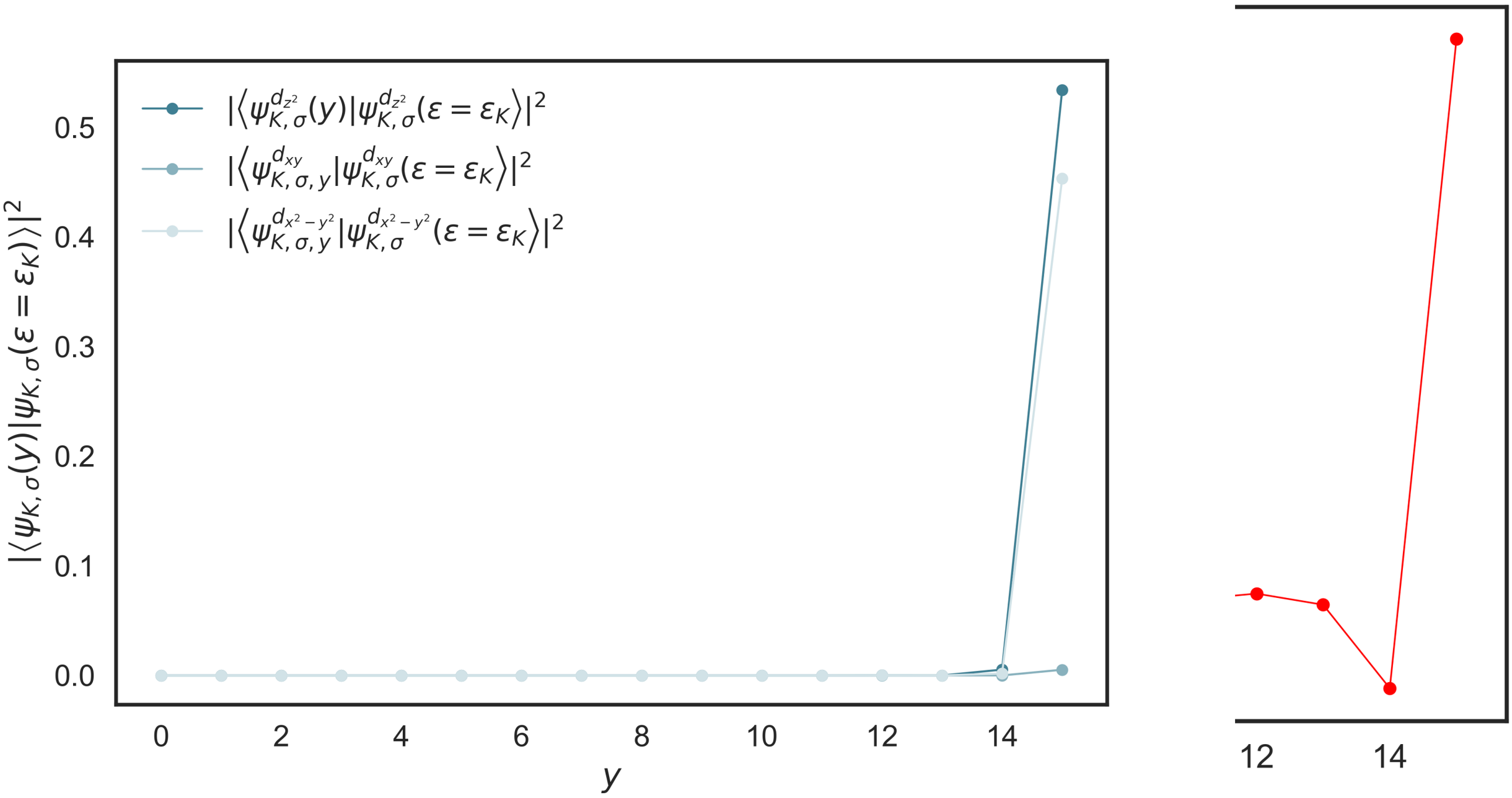
S^z along the transverse direction of the ribbon





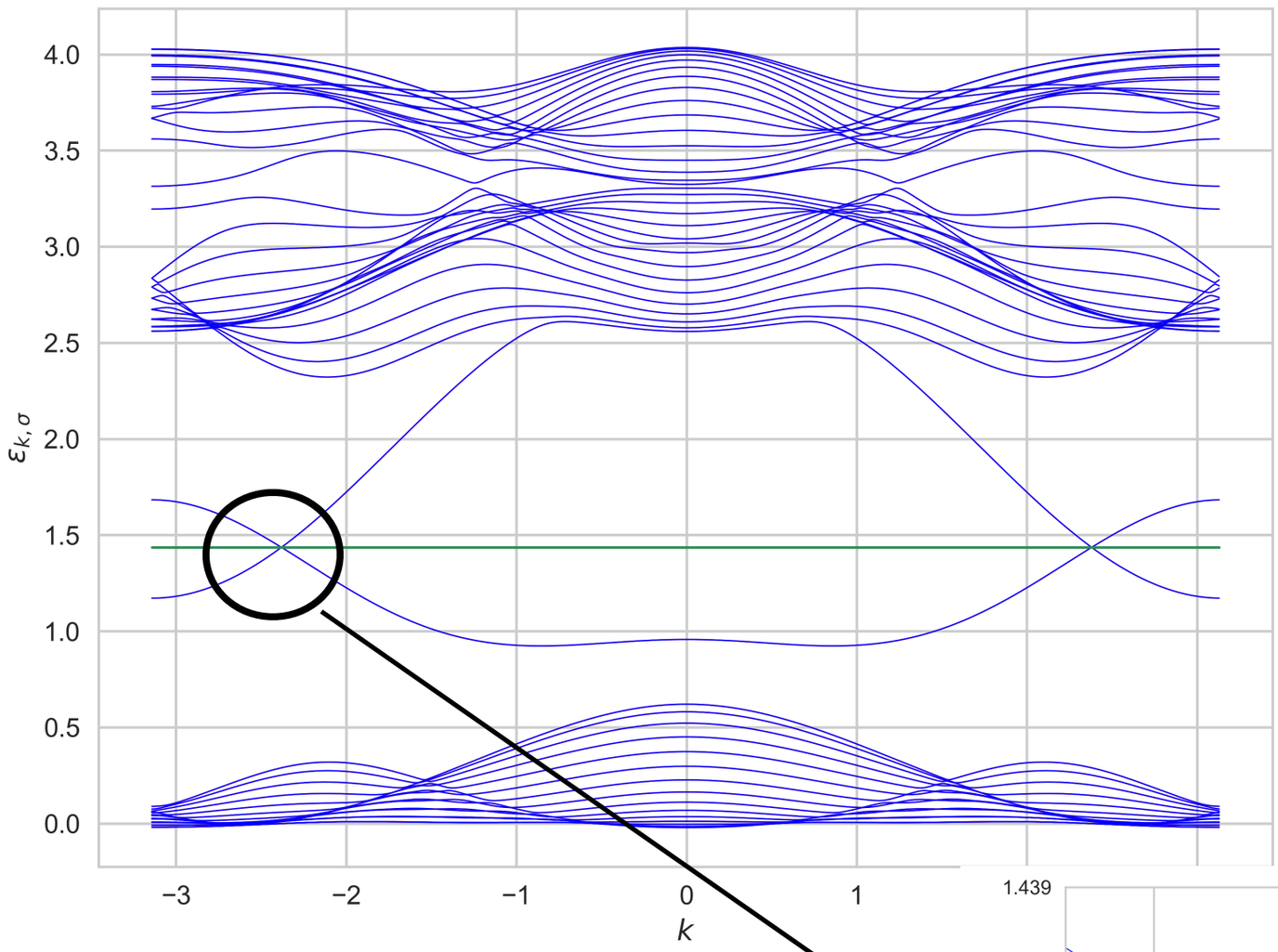
The edge-magnetism at the bottom is due to the edge states at the band crossing

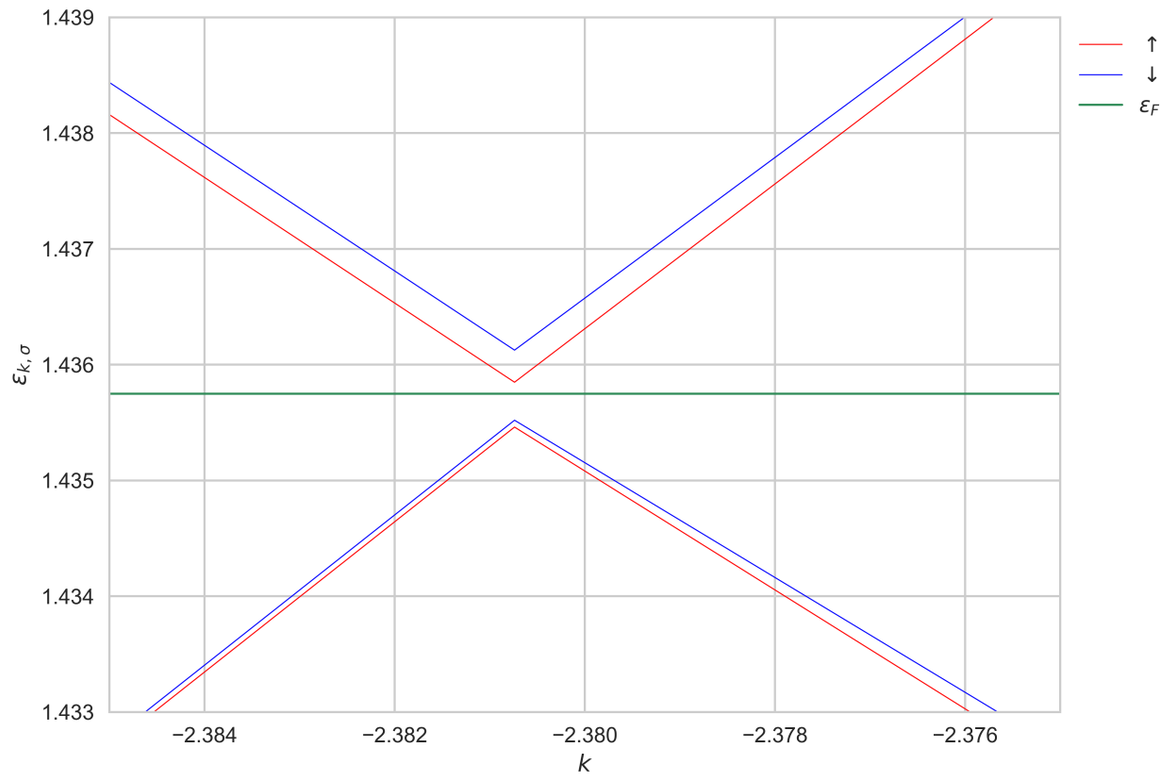
S^z along the transverse direction of the ribbon



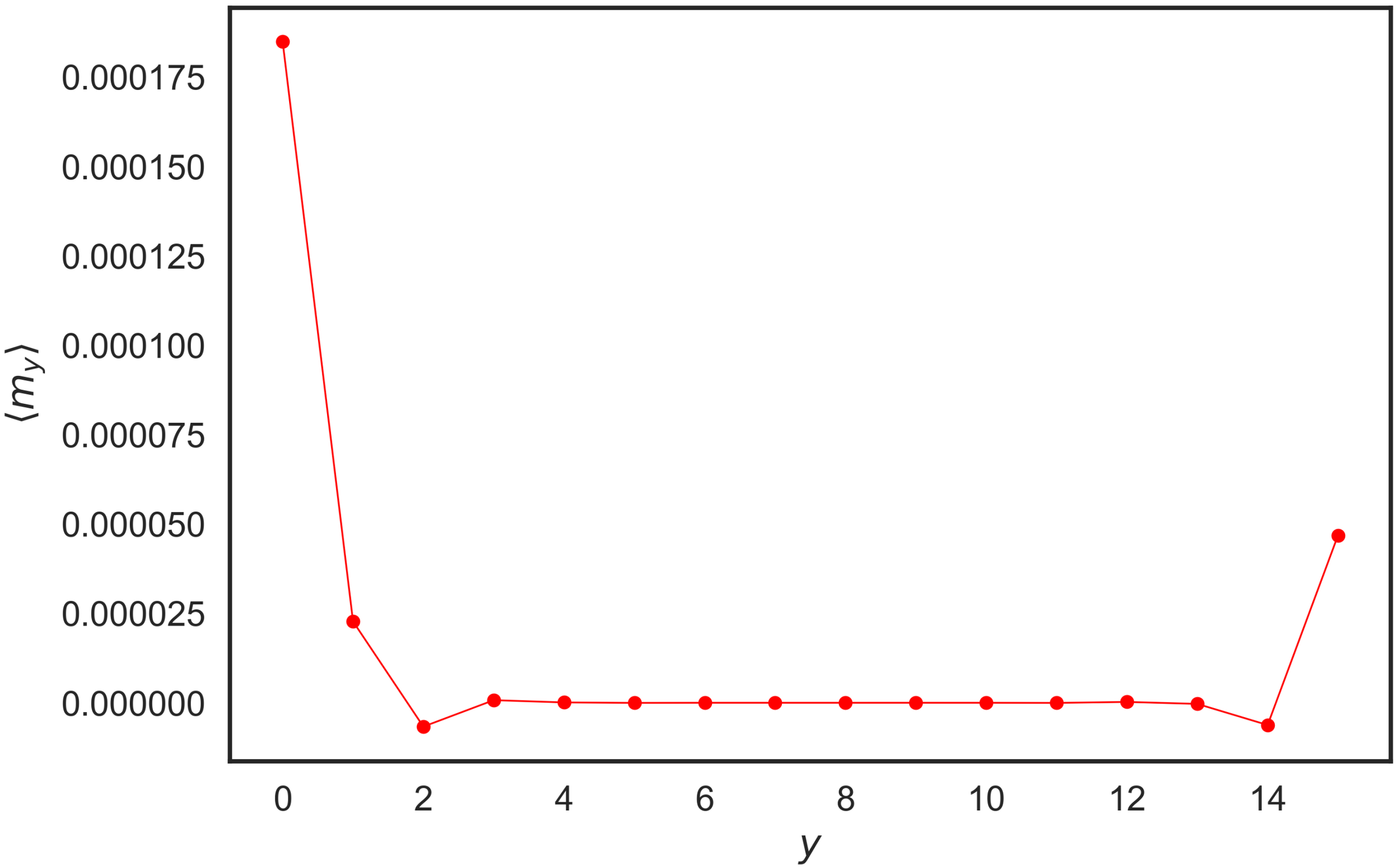
The edge-magnetism at the top of the sample is due to (spin-up) edge states at the K point.

For comparison, here's the band structure at U = 10

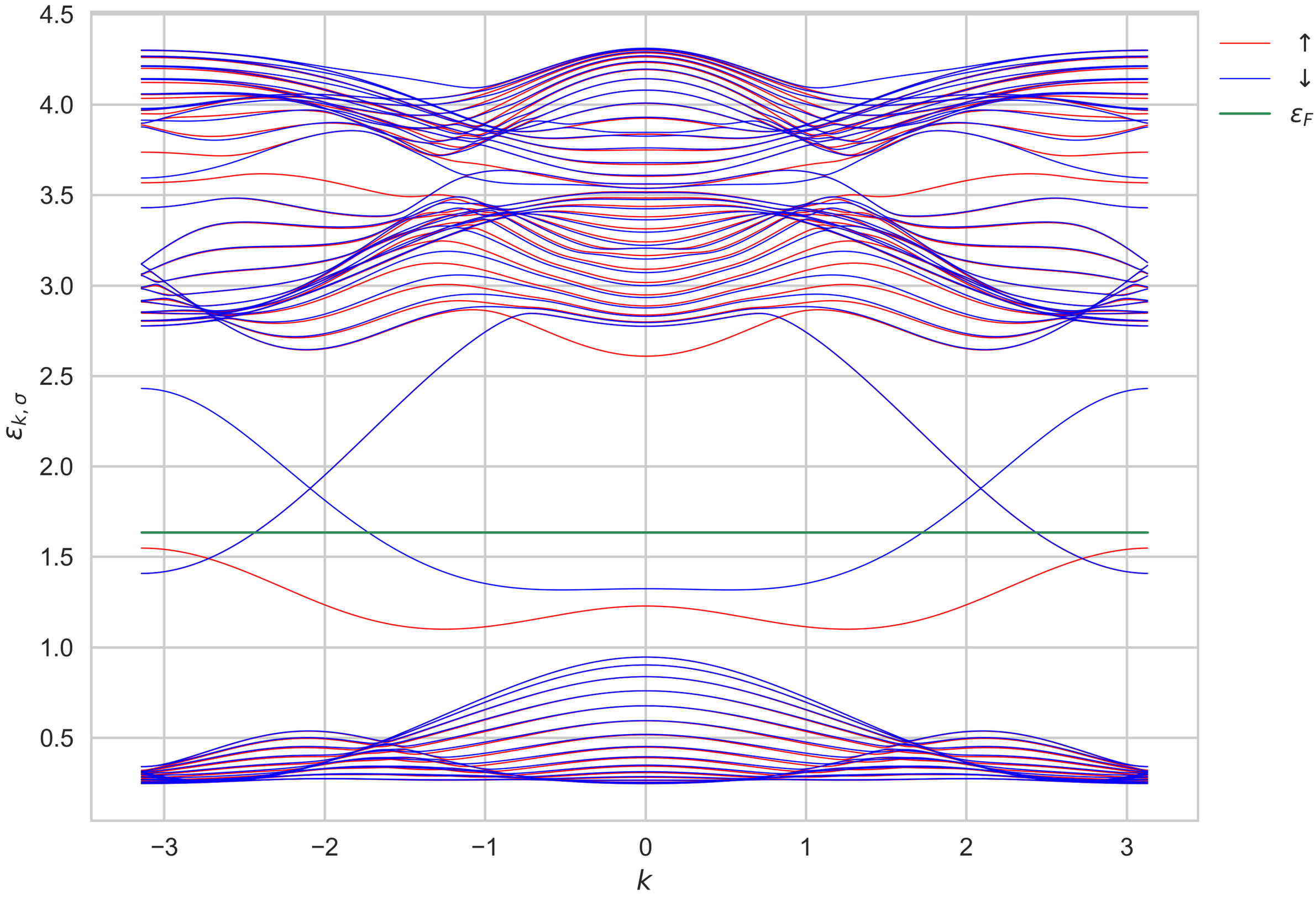




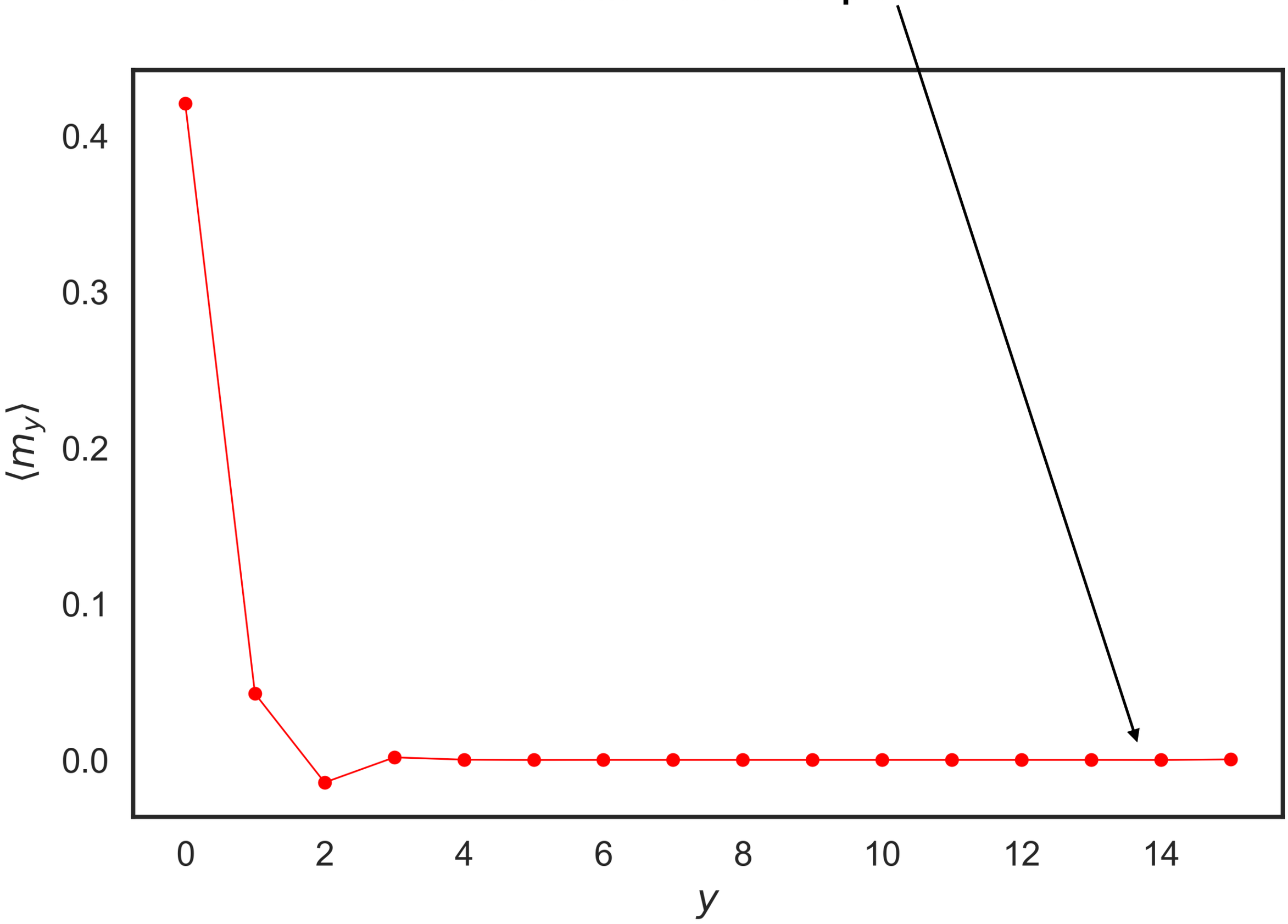
The slight lifting of the spin degeneracy leads to *nearly zero* edge magnetism



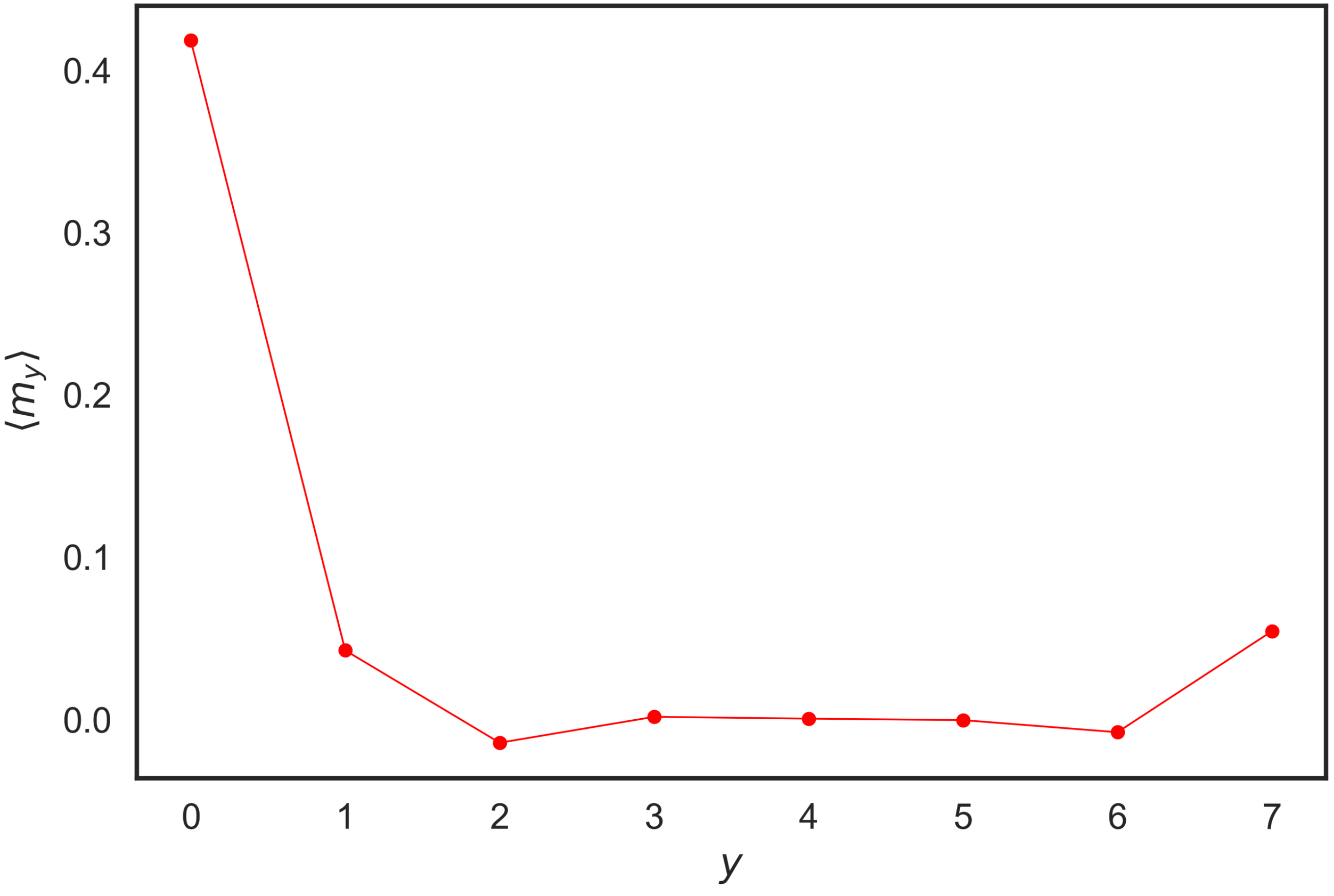
By U = 15, there is a significant K lifting and the shape of the bands changes



Edge-magnetism on the bottom of the sample appears, but the top remains unmagnetised. At some U between 15 and 20, band crossings lead to the magnetisation of the bottom of the sample.

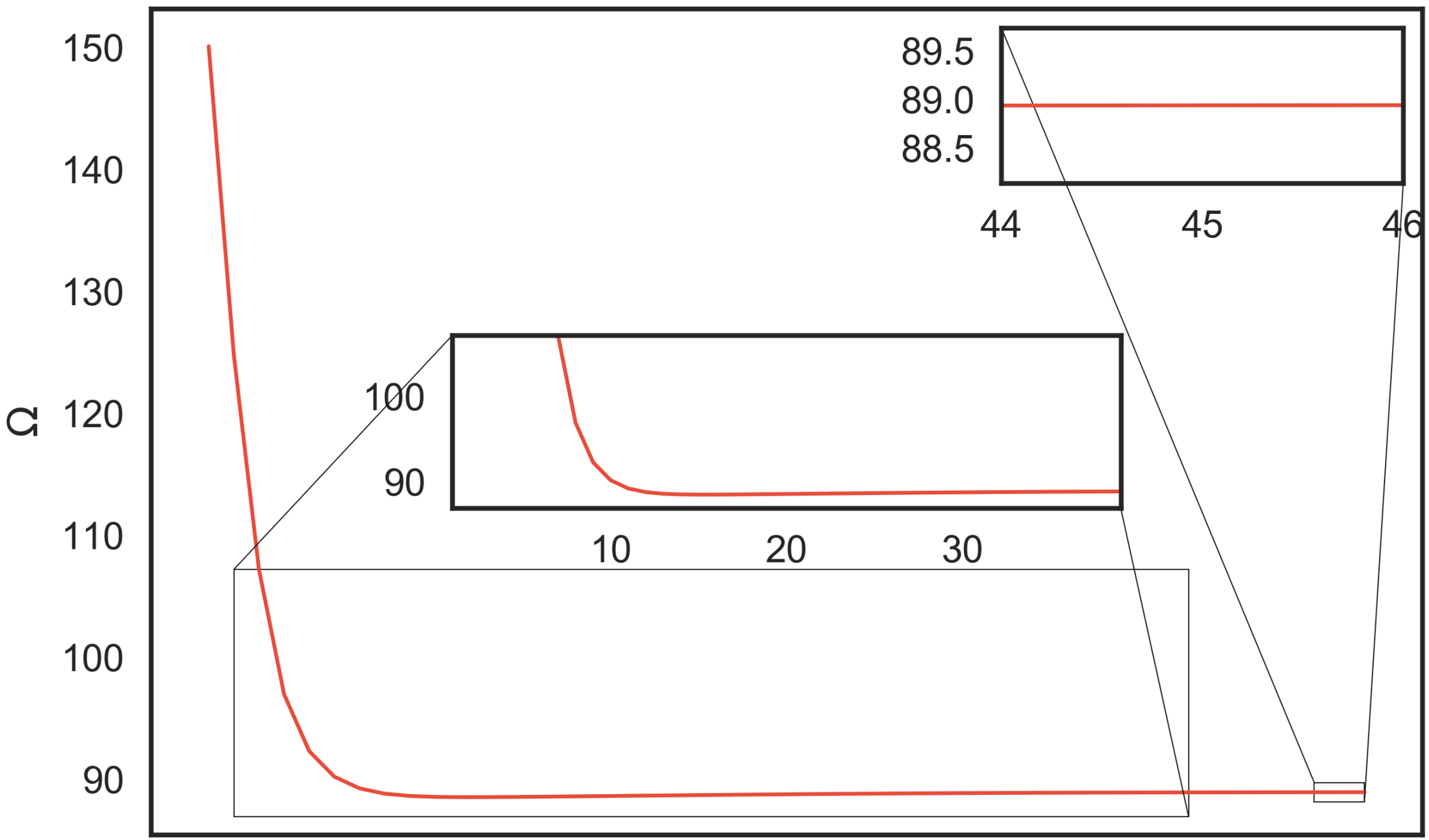


Even for a smaller system of width 8 at beta = 10, and with a small number of k's, we observe edge magnetism. It is stabilised at finite temperature for small systems

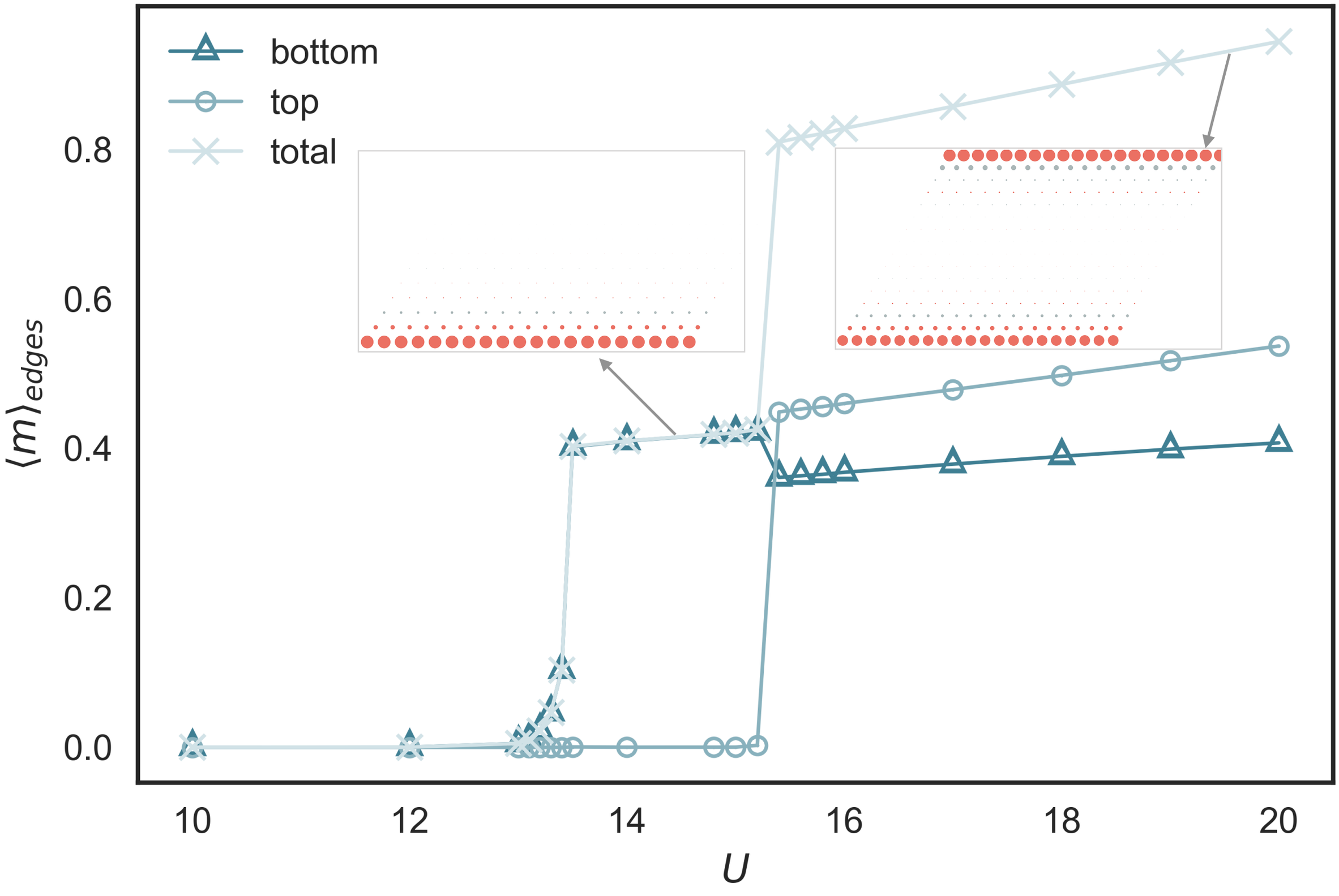


Grandpotential minimisation

$$N_x = 128\, N_y = 8\, U = 15\, \beta = 10$$

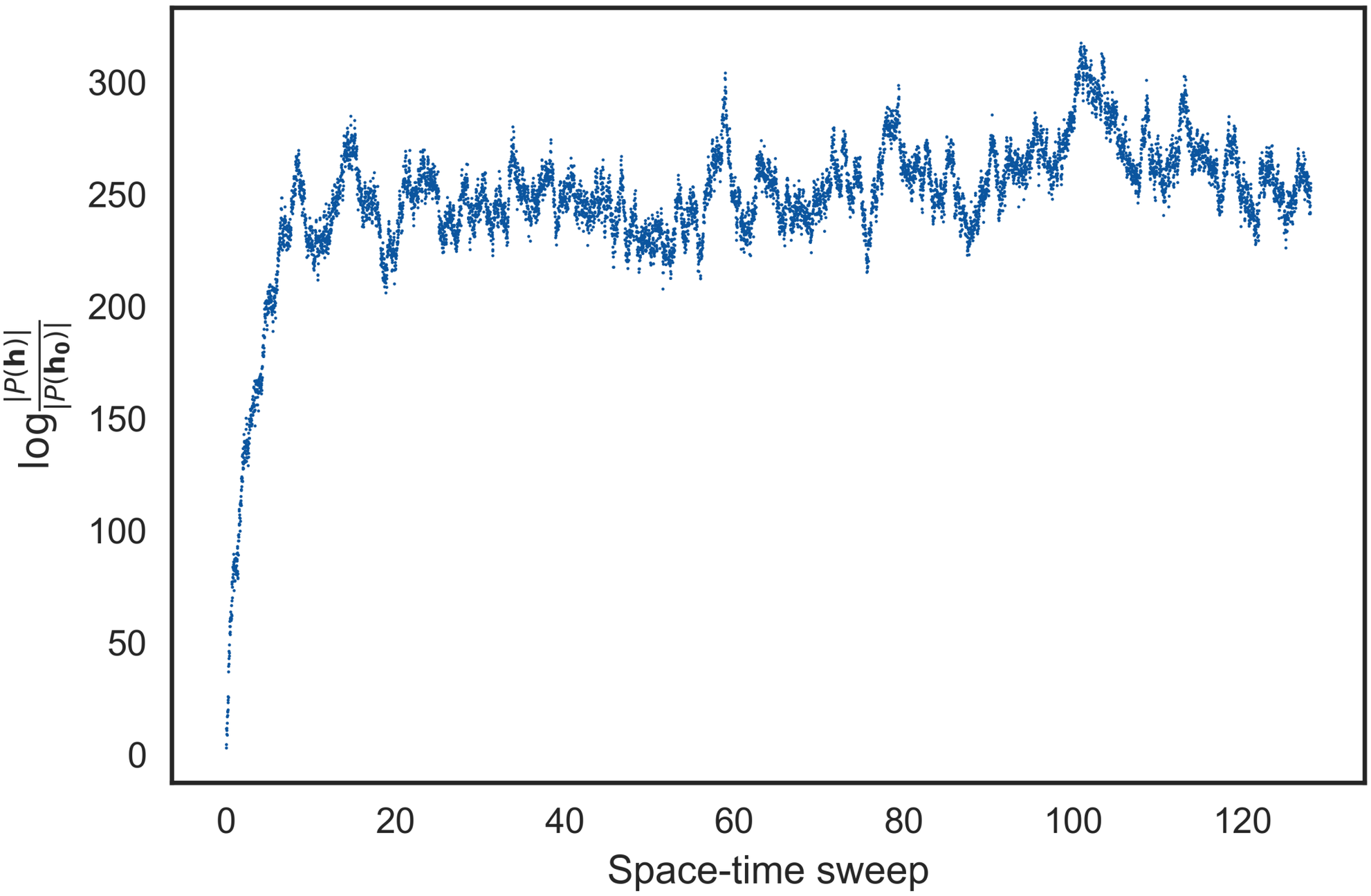


Phase transitions in MF



Preliminary QMC results

The algorithm converges for a (Nx, Ny) = (16, 8) ribbon (U=8, beta =4) :)



It appears that the simulation is giving edge magnetism (due to K lifting, but not due to band crossing?)