

1 Benchamrk week 6

Context: 30×15 SC with open boundary conditons.

We have a phase gradient of 117° . Starting from $\pi/2$. $T = 10^{-3}K$ and we iterrate until a relative change in both the real and imaginary part of Δ reach 0.001%.

1. Real guess of Δ and all parameters are free

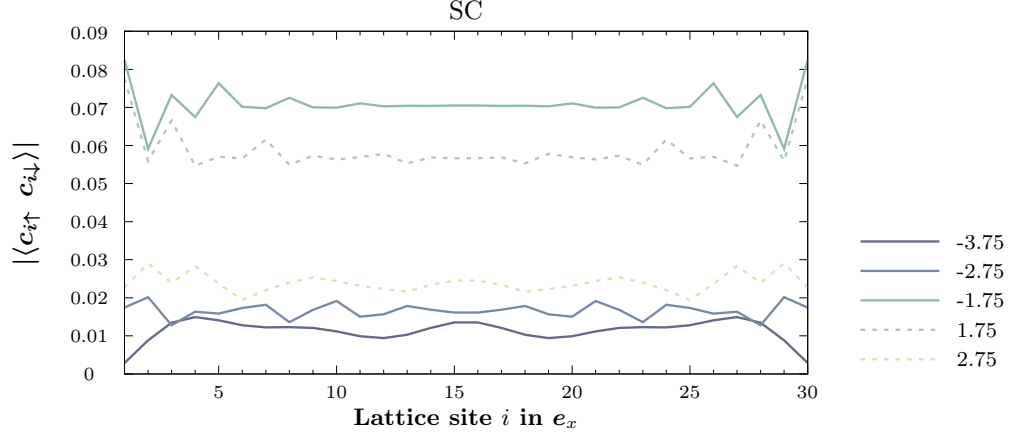


Figure 1

Here we can first denote unsymetric behaviour regarding the sign of μ . The value for the negative mu beeing higher than for their positive counterpart, we deduct that the Van Hove singularity has shifted towards the negative energies. Second the highest value where the algorithm doesn't converge towards zero is approx. 3.72 and the lowest is approx. -3.9, instead of the expected 4 and -4. So the density of state scales down on the energies and shifts itself to lower energies. From this we can read the following parameters

μ	-3.75	-2.75	-1.75	1.75	2.75	3.75
$ \langle c_{i\uparrow} c_{i\downarrow} \rangle _0$	0.01	0.018	0.07	0.058	0.025	diarded

2. Fixed norm of Δ on the side according to 1.

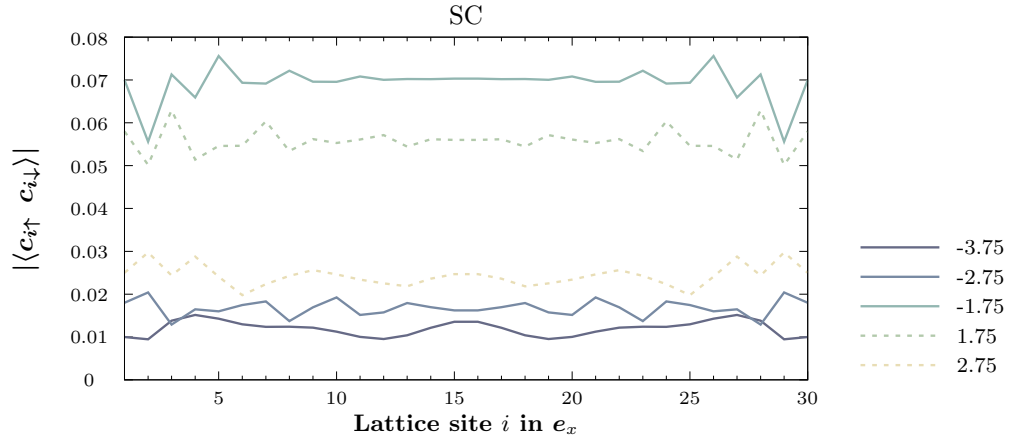


Figure 2

3.Fixed $|\Delta_0|$ and a phase of $\pi/3$ on the sides.

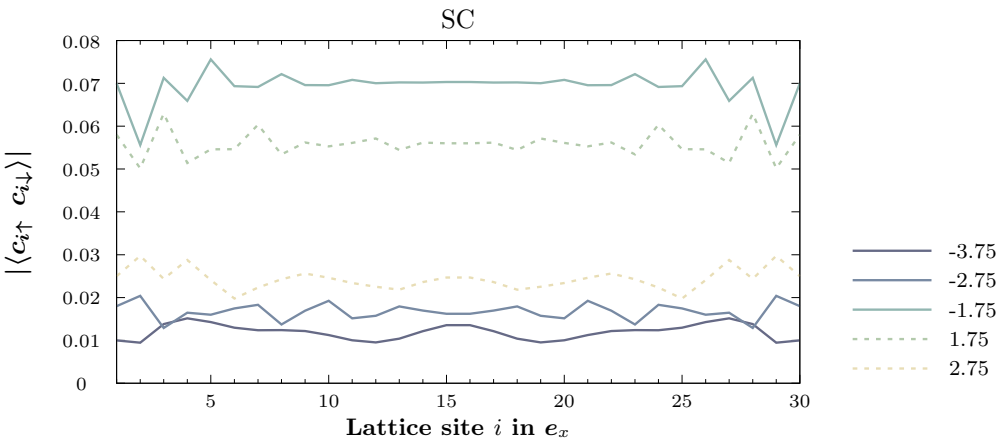


Figure 3

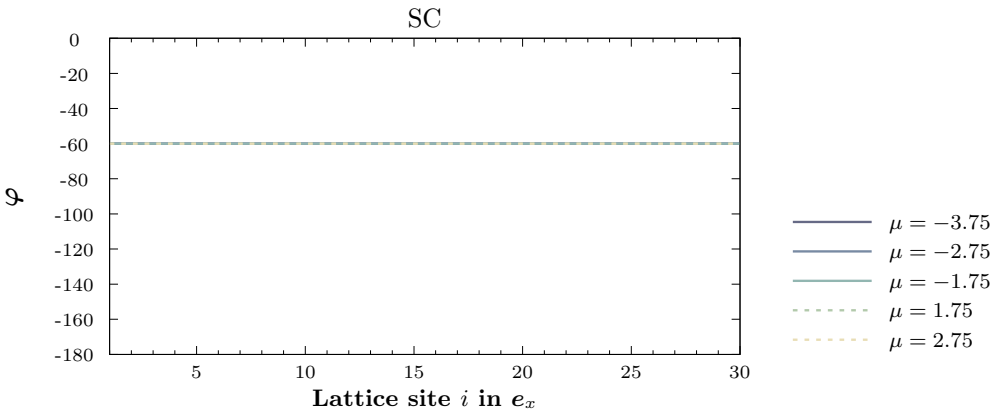


Figure 4

4.Fixed phase of $\pi/3$ on the sides left and a gradient of 117° .

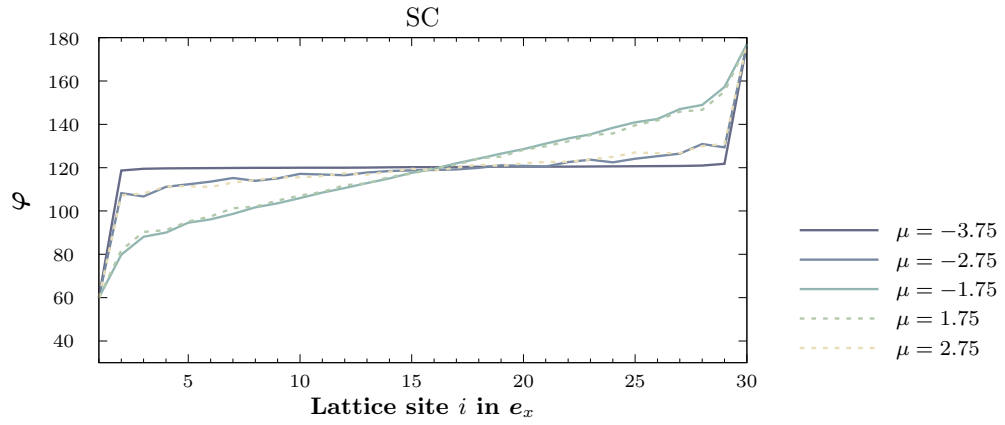


Figure 5: Using a start of $\pi/3$ on the sides and a gradient of 117deg.

And with a different starting phase:

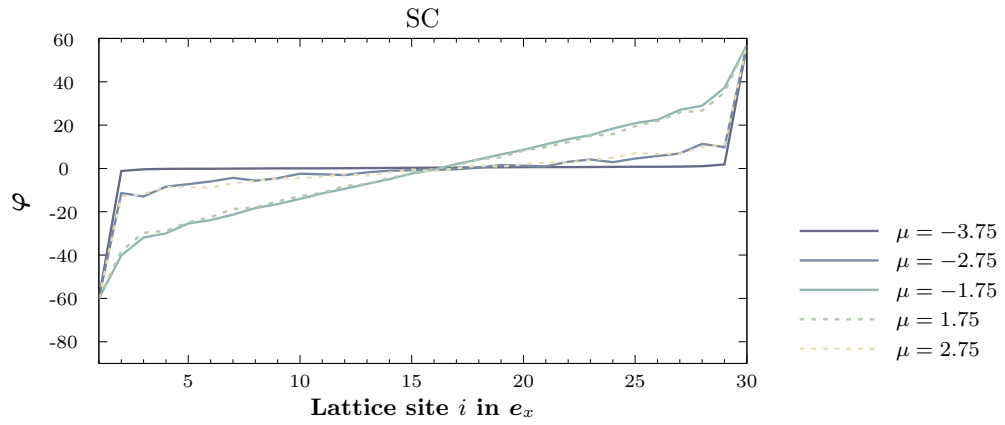


Figure 6: Using a start of $-\pi/3$ on the sides and a gradient of 117deg.

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5. Phase start independance of the gradient.

The current is independant of the phase, lets for instance take $\mu = -2.75$:

□ _____ □
¹./generateGraph.ps1 -GnuScript "gpScripts/Currents/Currents.long.SC.NoBC.gp" -
SimulationPath ". /SC30/NotFourier/FixedLinearPhaseGradient/Phase117deg/diffMU" -LatexPath
"/SC30/NotFourier/MeanLine.Phase/FixedLinearPhaseGradient/Phase117deg/allMU/starting -1.0472";

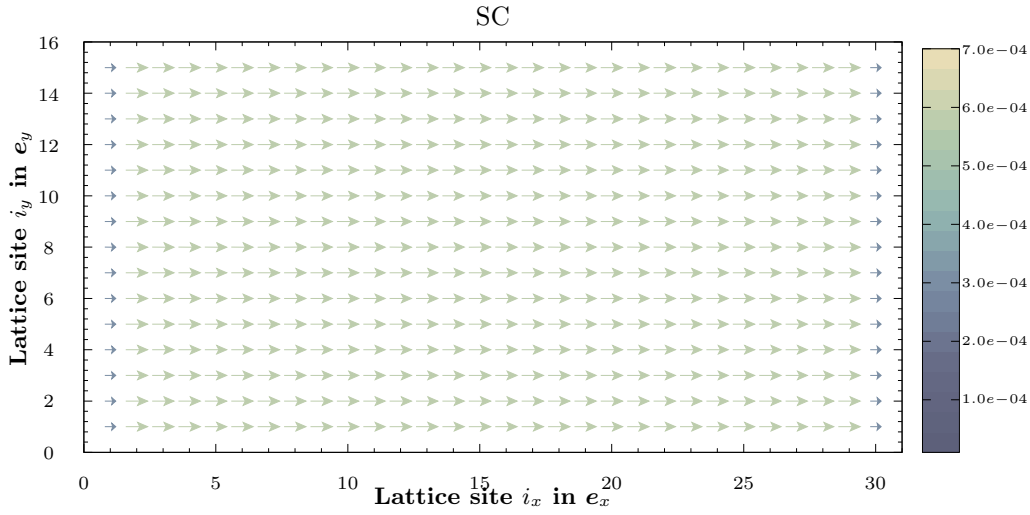


Figure 7: $\mu = -2.75$, using a start of $\pi/3$ on the sides and a gradient of 117deg.

And with a different starting phase:

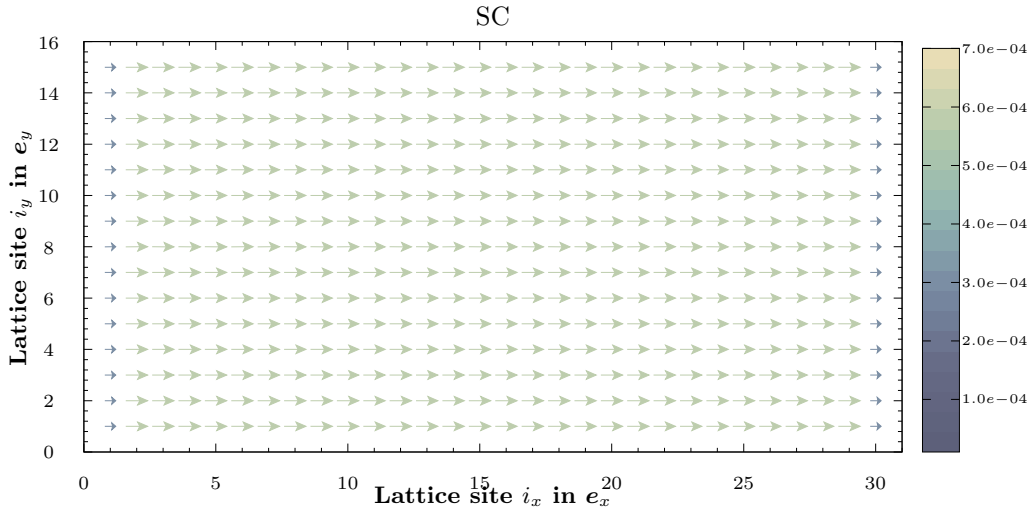


Figure 8: $\mu = -2.75$, using a start of $-\pi/3$ on the sides and a gradient of 117deg.

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As well as the continuity maps:

□ _____ □
²./generateGraph.ps1 -GnuScript "gpScripts/Currents/Currents_long_SC_NoBC.gp" -SimulationPath
"/SC30/NotFourier/FixedLinearPhaseGradient/Phase117deg/diffMU/-2.75/Starting_at/-1.0472" -LatexPath
"/SC30/NotFourier/Currents/FixedLinearPhaseGradient/Phase117deg/mu-2.75/starting_-1.0472/";

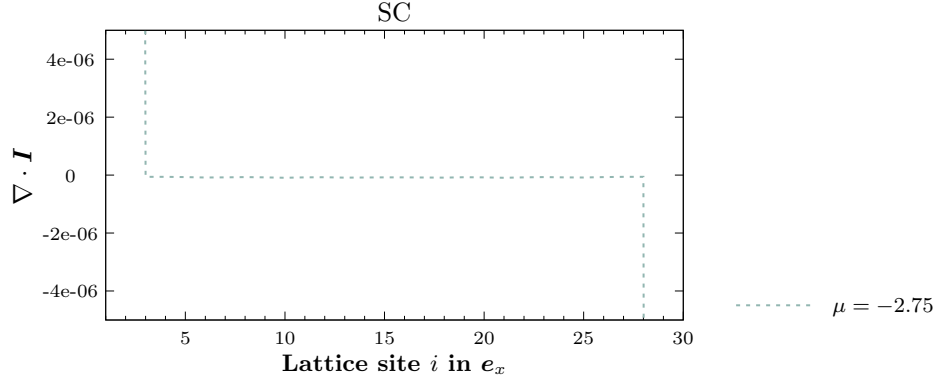


Figure 9: $\mu = -2.75$, using a start of $\pi/3$ on the sides and a gradient of 117deg.

And with a different starting phase:

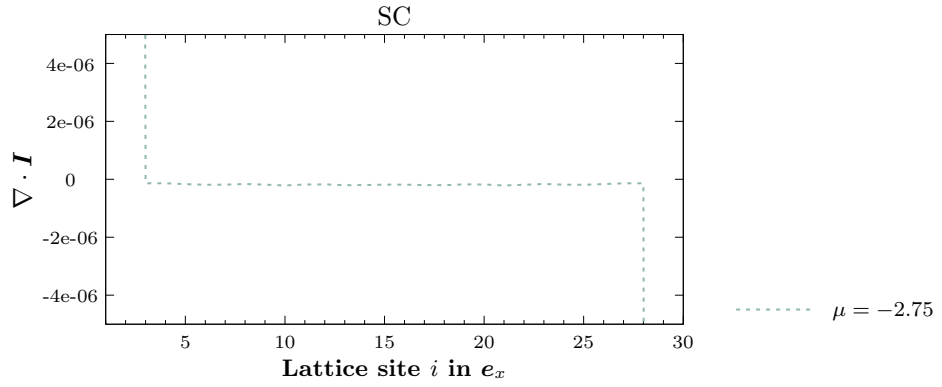


Figure 10: $\mu = -2.75$, using a start of $-\pi/3$ on the sides and a gradient of 117deg.

³ As we see the current conservation ∇I is three to four order of magnitude lower than the current itself. On the sides we have some huge drop. Recalling the fact that the current should be directly proportional to the phase gradient, having this sudden phase change on the sides results in drop of current which is then not conserved anymore. The way we look at the gradient in a discrete way is $\nabla f_i = (f_{i+1} - f_{i-1})/2a$. Here we setted a to one and we omitted the factor $\frac{1}{2}$. This means the plots represent $2\nabla f_i$. This explains why the current conservation ∇I has an opposite sign on each side of the lattice when we look at the current flow's direction. For exemple on the left we have $f_{i+1} > f_{i-1}$ so $\nabla f_i > 0$.

6. SC15AM15

□ _____ □
³./generateGraph.ps1 -GnuScript "gpScripts/MeanLine/MeanLine_continuity_long_SC.gp" -SimulationPath
"/SC30/NotFourier/FixedLinearPhaseGradient/Phase117deg/diffMU/-2.75/Starting_at/-1.0472" -LatexPath
"/SC30/NotFourier/Continuity/FixedLinearPhaseGradient/Phase117deg/mu-2.75/starting-1.0472/";

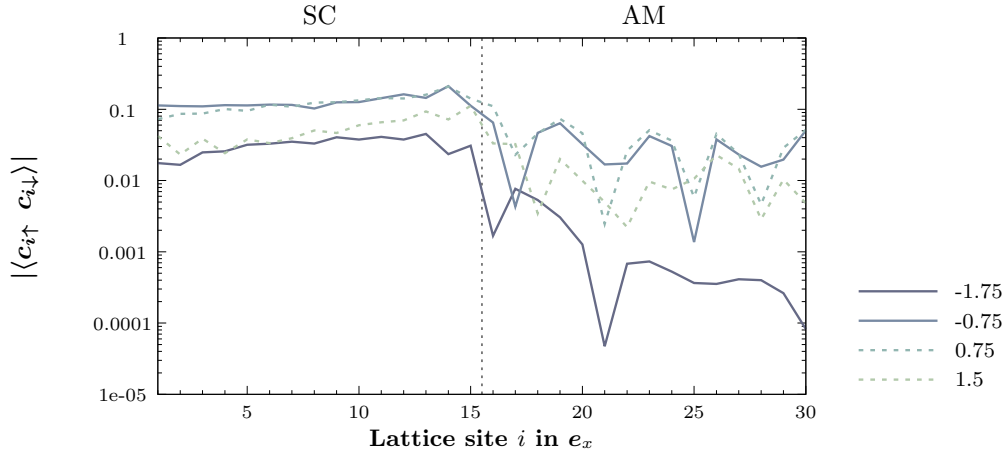


Figure 11: SC15AM15 with different μ .

The expectation value is very low ($< 10^{-6}$) for all values outer $-1.75 \leq \mu \leq 1.55$. We now stick with the lowest mu possible we can use, $\mu = -1.75$.

μ	-1.75	-0.75	0.75	1.5
$ \langle c_{i\uparrow} c_{i\downarrow} \rangle _0$	0.03	0.035	0.1	0.1

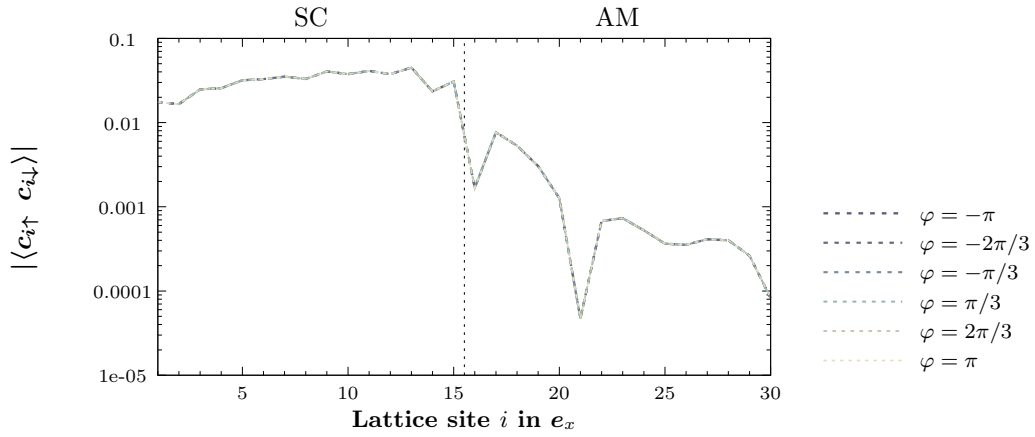


Figure 12: SC15AM15 with different μ .

For a normal metal we would expect these oscillations to vanish. Those are properties of the antiferromagnet. Instead we should just obtain an exponential decay.

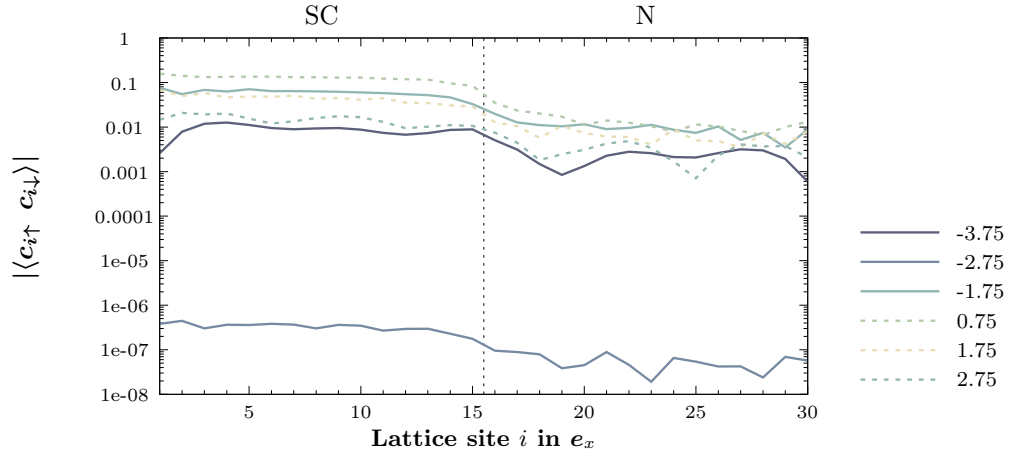


Figure 13: SC15N15 with different μ .

Here we have still observe some fluctuations but these are smaller than the oscillations we had by a factor ten. The lines are more recognisable for a high DOS, i.e. for small $|\mu|$. We see that $\mu = -2.75$ has an unnormal small value for a SC N. This is actely a statement that we are going to observe in the SC-AM-SC as well..

7. SC12-AM6-SC12

We first have a look at the tri layer SC over 12 sites followed by AM over 6 and another SC over 12.

The main change here is that having an SC on both sides we see the leaking effect of the SCAM setup described above taking place on each interface. These exponentiall oscillating decays meet eacother in the middle of the structure. The amplitude and frequency of the oscillations seams to be closely related to the μ value. We have a lot of noise in $\mu = 2.2$ despite the 200 iterrations which is relatively low compared to the other μ . Maybe the density of state is too low around this chemical potential.

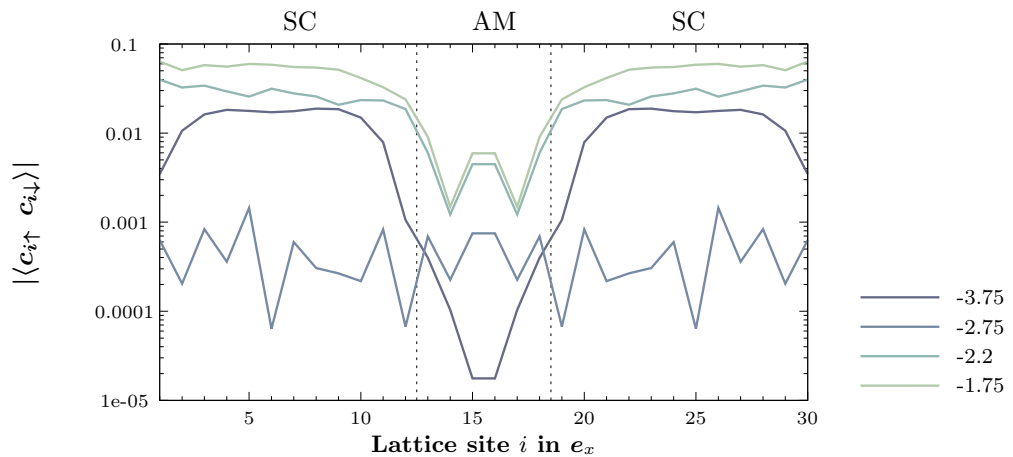


Figure 14: SC12AM6SC12 with $\mu = -3.75$ with a start at $\pi/3$

Now we can apply on constant phase everywhere and fix it on the sides. The simulation conserve that falt phase and it even drop to zero inside the AM.

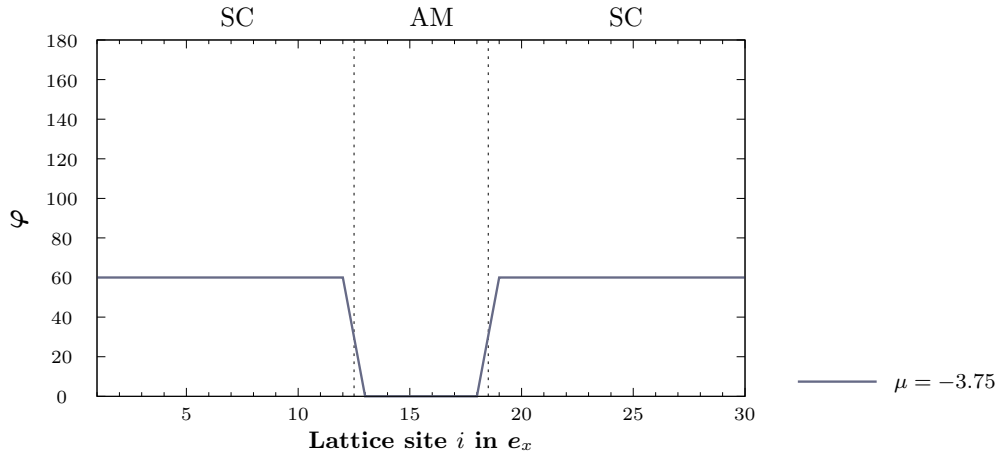


Figure 15: SC12AM6SC12 with $\mu = -3.75$ with a start at $\pi/3$

Currents for $\mu = -3.75$ In this section we want to show the phase gradient dependence of the current $I \propto \nabla\varphi$. We first fix the phase at $\pi/3$ on one side and initialize the system with a linear gradient of 117° over the system.

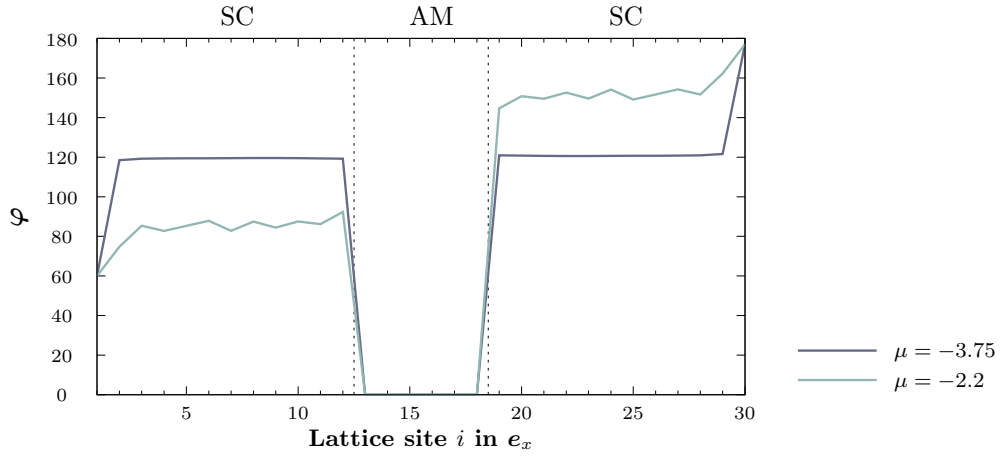


Figure 16: SC12AM6SC12 with $\mu = -3.75$ with a start at $\pi/3$

We see a dependence of the slope on the chemical potential as before [..].

Now we can inspect the current for these different values of μ .

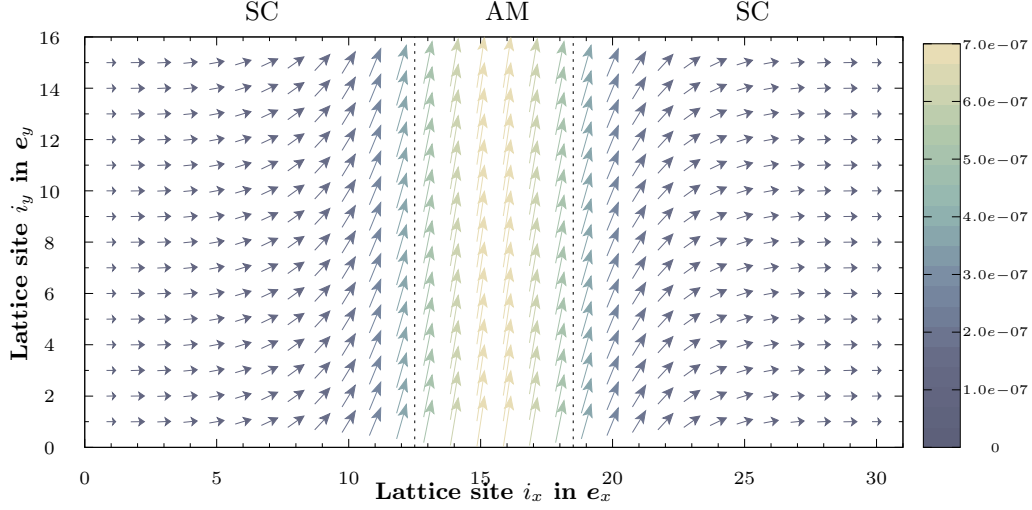


Figure 17: SC12AM6SC12 with $\mu = -3.75$ with a start at $\pi/3$

In this first case, the chemical potential is very low, which means that the density of state is low as well. Let us analyse the current following its natural flow. We start from the left, the phase gradient shows some current flowing to the right. The closer we get to the AM, the stronger its effect. We describe the AM as having a hopping of $t - m$ on the y axis and a hopping of $t + m$ on the x axis. These asymmetries can explain that the current has a perpendicular direction in the AM. After the AM we have the same behaviour than before. It is here important to note that due to the low μ the current in the SC is low, and is relatively high in the AM in comparison.

Beside those three major processes, we observe a smooth transition in the current between those different regions.

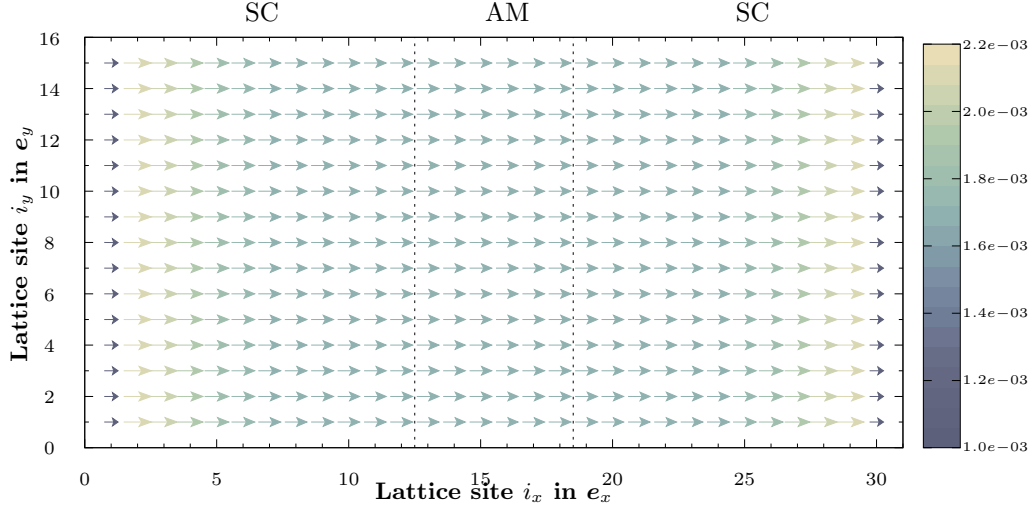


Figure 18: SC12AM6SC12 with $\mu = -2.2$ with a start at $\pi/3$

Now that we have increased the chemical potential, the density of state has increased as well. The current in the SC becomes much stronger by an order of magnitude of 10^4 . [Does the current in the AM scale accordingly with the μ ?]. Previous simulations have shown that with the slope of the phase gradient increases as well, resulting in a current that shadows the effects of the AM.

Now we can analyse the continuity of the current in both cases $\mu = -3.75$ and $\mu = -2.2$. Adding the AM seems to make the algorithm harder to converge. These results are obtained with 250 iterations and could be improved by increasing the number of iterations in a future work. At the moment an accuracy in relative change of $1.18e - 4\%$ is reached in the norm of Δ and one of 0.08% in the phase gradient (current). The main note we can take is that the continuity is about an order of magnitude lower than the current itself which is a relative poor result.

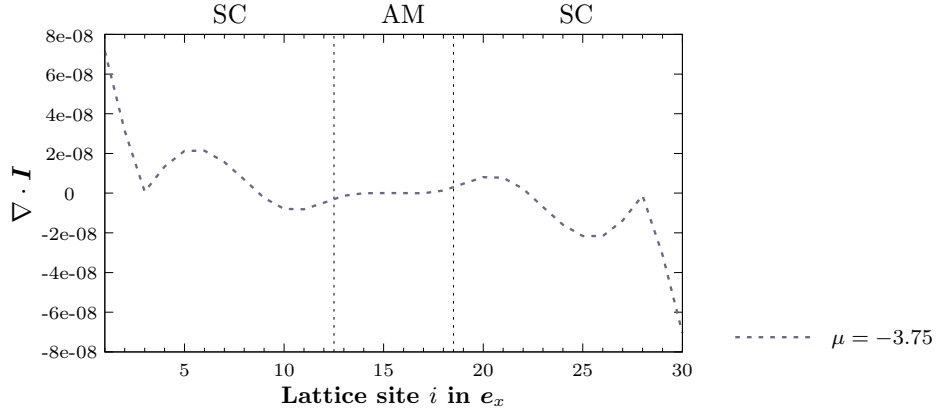


Figure 19: SC12AM6SC12 with $\mu = -3.75$ with a start at $\pi/3$

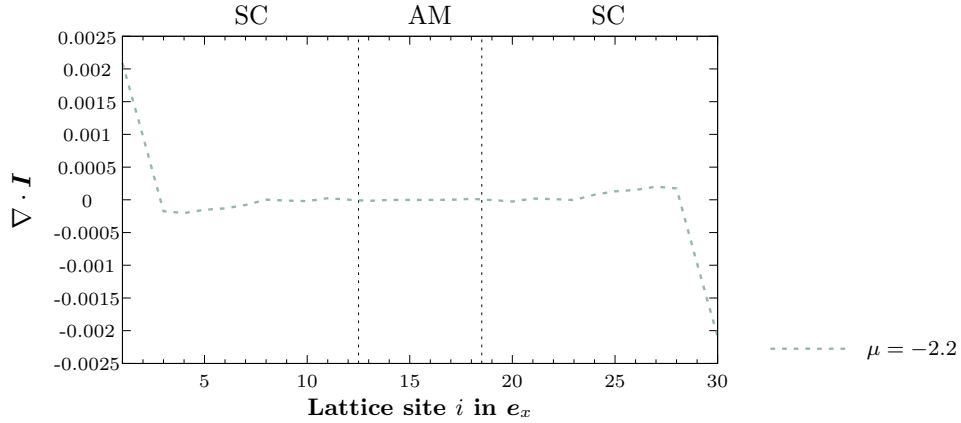


Figure 20: SC12AM6SC12 with $\mu = -3.75$ with a start at $\pi/3$

Leaving the current aside, we can make other observations. First we can try to have a better look at these oscillations. Here we have pictured them for different values of μ in a twice longer AM section than before. In the same way than for the Fig.14 and Fig.13 we see that we have a drop of the value for $\mu = -2.75$. Moreover for a $\mu = -3.75$ we see that the curve isn't symmetric anymore. Despite increasing the accuracy in the relative change, we are left with that curve. Maybe the oscillations regain amplitude and after leaking in the AM, it maybe regain some amplitude into the next SC. This hypothesis isn't very physical tho..

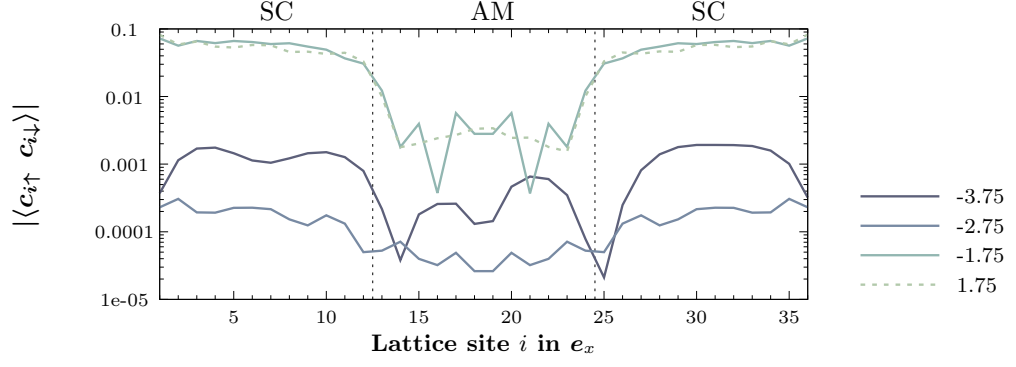


Figure 21: SC12AM12SC12 with $\mu = -3.75$ with a start at $\pi/3$

And lastly a rather important fact would be the phase independance of these oscillations. Here we plotted a given μ value for start constant phases over the system. We see that the curves are unchanged so that we get the same oscillations regardless the phase.

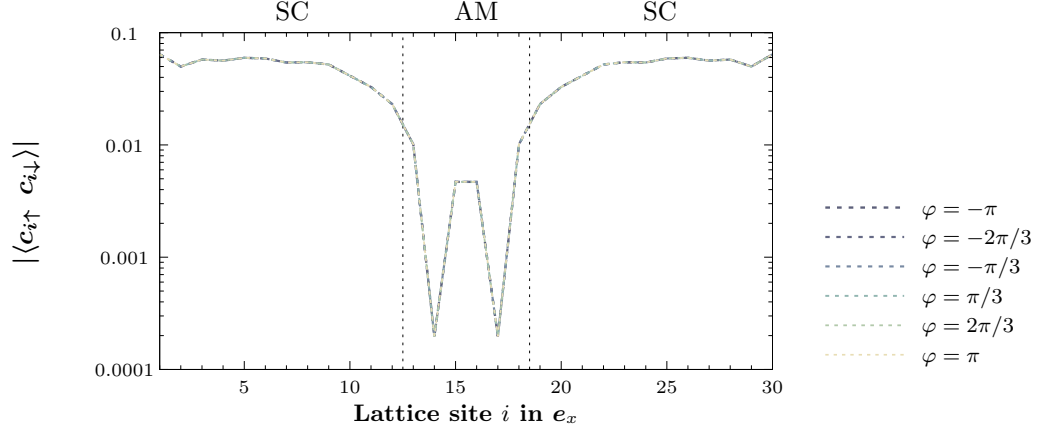


Figure 22: SC12AM12SC12 with $\mu = -3.75$ with a start at $\pi/3$