UNIVERSITY NAME (IN BLOCK CAPITALS)

Thesis Title

by

Author Name

A thesis submitted in partial fulfillment for the
degree of Doctor of Philosophy

in the

Faculty Name
Department or School Name

March 2018

Declaration of Authorship

I, AUTHOR NAME, declare that this thesis titled, 'THESIS TITLE' and the work presented in it are my own. I confirm that:

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UNIVERSITY NAME (IN BLOCK CAPITALS)

Abstract

Faculty Name
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Doctor of Philosophy

by Author Name

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

Acknowledgements

The acknowledgements and the people to thank go here, don't forget to include your project advisor...

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Abbreviations

LAH **L**ist **A**bbreviations **H**ere

Physical Constants

Speed of Light $c = 2.997\ 924\ 58 \times 10^8\ \mathrm{ms}^{-\mathrm{S}}$ (exact)

Symbols

a	distance	m
P	power	W (Js^{-1})
ω	angular frequency	$rads^{-1}$

For/Dedicated to/To my...

Chapter 1

Method

1.1 Data Generation

The evolution of the condensate phase was simulated using code written in C++. This defined the codensate as a square lattice consisting of N^2 points, where N is the linear size of the lattice, and each point restricted to be between $[0, 2\pi]$. Initially, the angle of each point was random, the system therefore being in the disordered phase. The simulation updated each lattice point according to the compactified and discretised equation:

$$\begin{aligned}\theta_{i,j}(t+\mathrm{d}t) = \theta_{i,j}(t) + \mathrm{d}t\,[&- D_x(\cos(\theta_{i,j}-\theta_{i+1,j}) + \cos(\theta_{i,j}-\theta_{i-1,j}) - 2) \\ &- D_y(\cos(\theta_{i,j}-\theta_{i,j-1}) + \cos(\theta_{i,j}-\theta_{i,j+1}) - 2) \\ &- \frac{\lambda_x}{2}(\sin(\theta_{i,j}-\theta_{i+1,j}) + \sin(\theta_{i,j}-\theta_{i-1,j})) \\ &- \frac{\lambda_y}{2}(\sin(\theta_{i,j}-\theta_{i,j-1}) + \sin(\theta_{i,j}-\theta_{i,j+1}))] \\ &+ 2\pi c_L \times \sqrt{\mathrm{d}t} \times \xi\end{aligned}$$

where $\theta_{i,j}(t)$ is the value of the condensate at points i, j of the lattice and $\mathrm{d}t$ is the timestep used. Periodic boundary conditions were used. The final term is the stochastic term where ξ is a uniformaly distributed random number (restricted to $[-0.5, 0.5]$) that was also added at each timestep. Finally, for all simulations D_x and D_y were set to 1 as the coordinates can always be rescaled to ensure this.

The timestep was initially chosen to be $\mathrm{d}t = 0.01$ and this was the value used to generate the significant data. However, other values were considered with: namely, $\mathrm{d}t = 0.02$ and $\mathrm{d}t = 0.001$ with system size 32. Figure. 1.1 comes the Binder cumulant for this system size for the three values of $\mathrm{d}t$. The evolution for $\mathrm{d}t = 0.02$ did not follow that of $\mathrm{d}t = 0.01$,

implying that $\mathrm{d}t = 0.02$ was potentially too large of a timestep, whereas the behaviour of $\mathrm{d}t = 0.01$ reasonably matched that of $\mathrm{d}t = 0.001$, demonstrating that $\mathrm{d}t = 0.01$ was an appropriate timestep for the simulation, and a smaller one was computationally unnecessary.

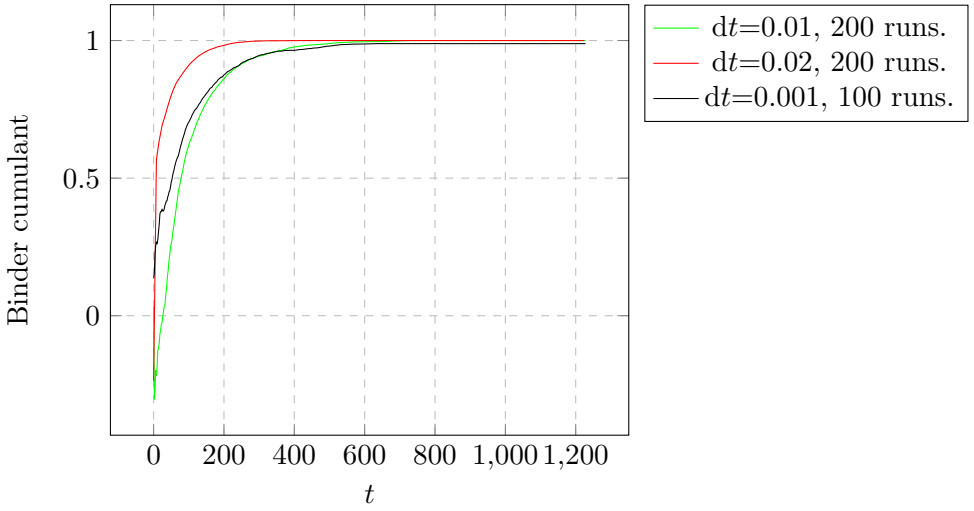

FIGURE 1.1: The Binder cumulant convergence for $L = 32$ at different values of $\mathrm{d}t$. The convergence of $\mathrm{d}t = 0.001$ compared to $\mathrm{d}t = 0.01$ suggests that a timestep of $\mathrm{d}t = 0.001$ was unnecessary, while the behaviour of $\mathrm{d}t = 0.02$ although qualitatively correct, deviated from that $\mathrm{d}t = 0.02$ significantly to be considered trustworthy.

The value of c_L at which the phase transition occurs was determined. Figure. 1.2 shows the number of vortices $t = 400$ for a system size of 64 at various values of c_L. The value $c_L = 0.2$ was then chosen for the remainder of project. For the value of $c_L = 0.1$ the Binder cumulant did not approach one at all in the case of $L = 128$, as shown in Figure. 1.3. This is likely a numerical artefact and can be explained by the existence of vortices stuck to lattice sites and not able to anihilate due to the low noise. The number of vortices is higher in Figure. 1.2 for $c_L = 0.1$ than higher values below the transition. XX shows a snapshat of the system for one realisation to illustrate this. This issue was also mentioned in XX.

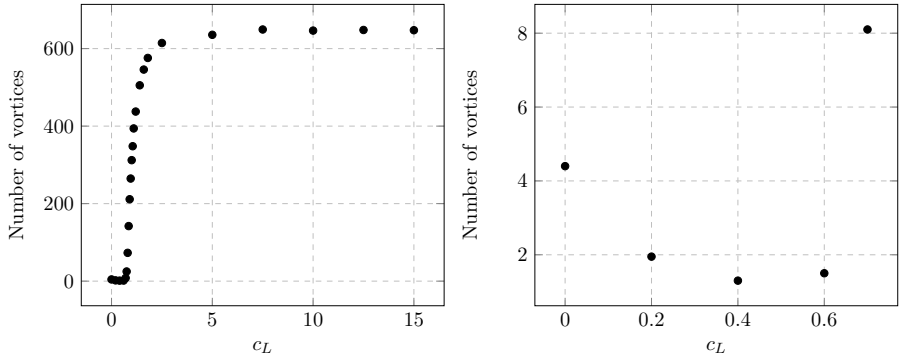

FIGURE 1.2: The number of vortices at the end of a simulation ($t = 400$) as a function of c_L for $L = 64$ with 20 runs.

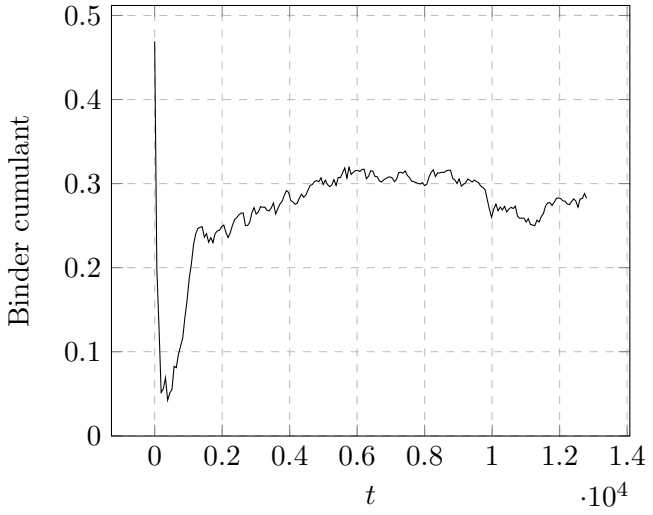

FIGURE 1.3: The Binder cumulant for $L = 128$ and $c_L = 0.1$. Despite being in the ordered phase, the Binder cumulant does not converge to near one due to the vortices.

1.2 Data Extraction

Using the generated data, the Binder cumulant was calculated as follows: for each timestep of a simulation, the magnetisation $\boldsymbol{M}$, defined by

$$\boldsymbol{M} = \frac{1}{N^2}\sum_{i,j}(\cos(\theta_{i,j}), \sin(\theta_{i,j})),$$

where the sum is over all lattice points, was calculated. The averages (over all the realisations) $\left\langle \boldsymbol{M}^2 \right\rangle$ and $\left\langle \left(\boldsymbol{M}^2\right)^2 \right\rangle$ were then used in the Binder cumulant given by

$$g = 2 - \frac{\left\langle (\boldsymbol{M}^2)^2 \right\rangle}{\left\langle \boldsymbol{M}^2 \right\rangle^2}$$

To estimate the error, the Binder cumulant was considered to be a function of the variables $\boldsymbol{M}^2 >$, i.e.

$$g = 2 - N\frac{\sum_i (\boldsymbol{M}_i^2)^2}{\left(\sum_i \boldsymbol{M}_i^2\right)^2}$$

where the sum is over every realisation and N is the number of realisations. These variables are indentical and independent, so the error of each is the same and is approximated by

$$\sigma^2_{\boldsymbol{M}^2} = \frac{1}{N-1}\sum_i (\boldsymbol{M}_i^2 - \left\langle \boldsymbol{M}^2 \right\rangle)^2 = \frac{N}{N-1}(\left\langle (\boldsymbol{M}^2)^2 \right\rangle - \left\langle \boldsymbol{M}^2 \right\rangle^2).$$

Using error propagation, the error on the Binder cumulant is

$$\begin{aligned}
\sigma_g^2 &= 4N^2 \sum_k \left(-\frac{\boldsymbol{M}_k^2}{\left(\sum_i \boldsymbol{M}_i^2\right)^2} + \frac{\sum_i (\boldsymbol{M}_i^2)^2}{\left(\sum_i \boldsymbol{M}_i^2\right)^3} \right)^2 \sigma_{\boldsymbol{M}^2} \\
&= \frac{4N^3}{N-1} \left(\left\langle (\boldsymbol{M}^2)^2 \right\rangle - \left\langle \boldsymbol{M}^2 \right\rangle^2 \right) \sum_k \left(\frac{(\boldsymbol{M}_k^2)^2}{\left(\sum_i \boldsymbol{M}_i^2\right)^4} + -2\frac{\boldsymbol{M}_k^2 \sum_i (\boldsymbol{M}_i^2)^2}{\left(\sum_i \boldsymbol{M}_i^2\right)^5} + \frac{\left(\sum_i (\boldsymbol{M}_i^2)^2\right)^2}{\left(\sum_i \boldsymbol{M}_i^2\right)^6} \right) \\
&= \frac{4N^3}{N-1} \left(\left\langle (\boldsymbol{M}^2)^2 \right\rangle - \left\langle \boldsymbol{M}^2 \right\rangle^2 \right) \left(\frac{N \left\langle (\boldsymbol{M}^2)^2 \right\rangle}{N^4 \left\langle \boldsymbol{M}^2 \right\rangle^4} - 2\frac{N^2 \left\langle \boldsymbol{M}^2 \right\rangle \left\langle (\boldsymbol{M}^2)^2 \right\rangle}{N^5 \left\langle \boldsymbol{M}^2 \right\rangle^5} + \frac{N^3 \left\langle (\boldsymbol{M}^2)^2 \right\rangle^2}{N^6 \left\langle \boldsymbol{M}^2 \right\rangle^6} \right) \\
&= \frac{4}{N-1} \left(\left\langle (\boldsymbol{M}^2)^2 \right\rangle - \left\langle \boldsymbol{M}^2 \right\rangle^2 \right)^2 \frac{\left\langle (\boldsymbol{M}^2)^2 \right\rangle}{\left\langle \boldsymbol{M}^2 \right\rangle^6}
\end{aligned}$$

which is proporiotnal to $1/N$, as expected.

To calculate the number of vortices or anti-vortices, we use a discretised version of their defining equation. The 'loop', starting at a point $\theta_{i,j}$, is the path

$$\theta_{i,j} \to \theta_{i+1,j} \to \theta_{i+1,j+1} \to \theta_{i,j+1} \to \theta_{i,j}$$

and the value of one angle minus the value of the previous angle is calculated and all such differences are summed. If the total is greater than or equal to 2π, there is a vortex, whereas if the total is less than or equal to -2π, there is an antivortex.

The uncertainty on the number of vortices was unfortunately not calculated as the necessary data for larger system sizes had to be periodically deleted and the need for the vortex uncertainty was not considered (in fact it was fortuotous that the uncertainty on the Binder cumulant was calculable without requiring extra data). That being said, there are indications that such an error would would be small based on the variation of the average number of vortices vs the number of realisations, as in Figure. **??**. Here it is plotted for the $L = 128$ linear case at snapshot 10. This was chosen as the largest system size and the most realisations for the size. There is clearly a downward trend, but the relative variation $\sim 0.15/4.725 = 0.03$ or 3% which is not extreme. It is not acceptable for exact values but should be acceptable to observe general trends and also in the comparison to the expectation in the linear case. To calculate the uncertainties, we used Python's `scimpy` package.

For calculating the correlation functions, the average of $\cos(\theta_{i,j} - \theta_{i,0})$ was calculated from $i = 0$ to $i = L - 1$ and over all realistations at a specific time step. The correlation distance is given by j and $j = 1$ to $j = L/2$ was used.

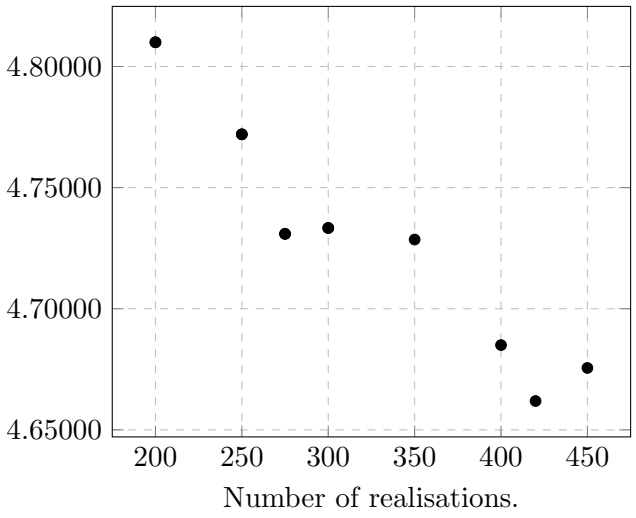

FIGURE 1.4: The number of vortices as a function of the number of realisatations for $L = 128$ and $\lambda_x = \lambda_y = 0$ at snapshot 10.