COMSOL MULTIPHYSICS

Two-dimensional superconductor in uniform magnetic field

-Analysis of Abrikosov lattice in type II superconductor

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1. INTRODUCTION

1.1. Abstract

In this work, the vortex nucleation process in a mesoscopic superconductor with different geometry is numerically investigated in terms of time dependent Ginzburg– Landau theory. We solved the equations simultaneously for different initial parameters. The influence of the magnetic field on the number of vortices was tested and further analysed. Although all parameters are temperature dependent, in this study it was chosen to be $T = 0$, therefore no critical temperature could be established. The main goal of this study is to show the reader the impact of defects in different geometries in comparison to ideal geometries. Through the whole simulation the parameters are chosen as follows: $\kappa = 4, \sigma = 1$, unless stated otherwise.

1.2. Theoretical model

Challenging world of high temperature superconductors has proven that microscopic theories such as BCS, which undeniably pushed the science of superconducting states a huge step further and proven to describe a vast majority of type I superconductors, proceeded to fail to clearly develop a prediction and model explanation of them. There were many attempts but rather no commonly accepted theory has emerged for many years so. After that, many thought to improve the BCS itself because of the formulation of the Green functions used. There were a lot of quasi-classical methods which have worked, despite they weren't event meant to do so. Nevertheless, the main problem in creating a microscopic theory is that we shall deal with non-equilibrium response to applied fields and not only nonstationary behaviour of the quantum states.

For that so, in many purposes, the quasi-classical Ginzburg-Landau theory with a time dependent dynamics is a powerful tool to describe kinetics of superconductors within a certain limits. Mainly because it leaves a microscopic theory behind and leaves us with properties of the system as a whole, which is a lot easier to describe.

The fact is that the dynamics of vortices controls almost all of the magnetic properties in type II SC, especially the high temperature ones.

The most important parameter in our theory would be a order parameter, which is proportional to the wave function of superconducting electrons (as BCS theory has also proven). As the electrons couple via many complex interactions in the superconductor, especially a repulsive *Coulomb* force, they do form a *Bose condensate*. The parameter is of course the normalised, complex function with the same phase for all particles in the condensate in equilibrium state, without current. The phase only changes if the symmetry for the condensate does change, clearly when the supercurrent is present.

Thus, there exists a coherent phase for all of the electrons in the condensate.

$$\Delta = |\Delta| e^{i\chi}$$

As in all of physical states, we shall also consider a single particle excitation with a gap:

$$\epsilon_p = \sqrt{\xi_p^2 + |\Delta|^2}$$

so all excitations have energies above $|\Delta|$.

The Ginzburg-Landau theory(G&L 1950) deals with second order phase transitions. We start with a phenomenological theory with fundamental assumptions:

a) **There exists a complex, scalar order parameter ψ (Δ, as we stated above)**

b) **There exists a homogeneous free energy(F) density, which can be expanded in a power series of an order parameter**

c) **The coefficients of the expansion are functions of a absolute temperature**

$$F = F_n + \alpha(T)|\psi^2| + \frac{\beta(T)}{2}|\psi^4|$$

with an assumption that the equation is valid near critical temperature. $\alpha \sim (T - T_c)\alpha_0, \beta(T) \sim \beta_0 = const$

The order parameter has an absolute minimum $-\frac{\alpha}{\beta} \neq 0$ when $T < T_c$ and 0 when it is above. It poorly describes the effects rather distant from T_c and in the T_c itself. The free energy expansion is supplemented with Maxwell equations for magnetic field. It predicts in momentum that the Cooper pair would have a double charge for both electrons. When we include magnetic potential.

$$\boldsymbol{p} = -ih\boldsymbol{\nabla} - \frac{2e}{c}\boldsymbol{A}$$

We can easily provide study of Gibbs energy:

$$E(\psi, \boldsymbol{A}) = \int_\Omega F + \frac{1}{2m^*}\left|\left(-ih\boldsymbol{\nabla} - \frac{2e\boldsymbol{A}}{c}\right)\psi\right|^2 + \frac{|\boldsymbol{\nabla} x\boldsymbol{A} - \boldsymbol{H}|^2}{8\pi}$$

After the standard procedure of energy minimalization we have corresponding, stationary Landau equations:

$$\begin{cases} \frac{1}{2m^*}\left(-ih\nabla - \frac{2e\boldsymbol{A}}{c}\right)^2 \psi + \alpha\psi + \beta|\psi|^2\psi - 0 \\ \frac{\nabla\mathrm{x}(\nabla\mathrm{x}\mathbf{A})}{4\pi} = \frac{j}{c} = \frac{2eh}{2im^*c}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{(2e)^2}{m^*c^2}|\psi|^2\boldsymbol{A} \end{cases}$$

With corresponding boundary conditions(notice that the **H** is only the outside magnetic field and $\nabla x A$ doesn't imply it being equal H):

$$\boldsymbol{p}\psi \cdot \boldsymbol{n} = 0 \quad \nabla x\boldsymbol{A} = 0$$

Which is inconvenient and therefore , we make a variation of Gibbs energy putting $\nabla x H$ to the equation, which gives us real boundary condition of $\nabla x A = H$.

We then put the remark that the vortices(very briefly, rapid changes of order parameter) tend to meet the boundary of the sample perpendicularly. Thus, as the circulating supercurrents form the vortex, It generates magnetic field tangential of the core, and perpendicular to the sample boundary.

Then we put a gauge transformation in the presence of magnetic field.

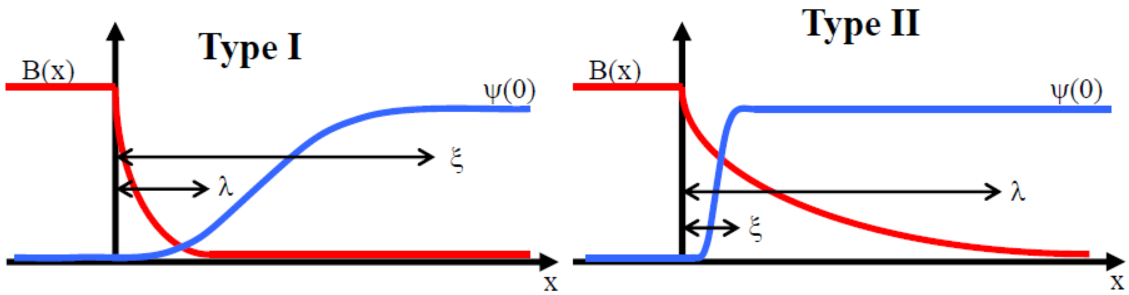
We have two particular solutions.

a) $\psi = 0$ and standard rotation, when H(applied field) is large.

b) $\psi = \psi_0 = \sqrt{\left|\frac{\alpha}{\beta}\right|}$ and **A**=0 when **H**=0. This is pure superconducting state without field applied.

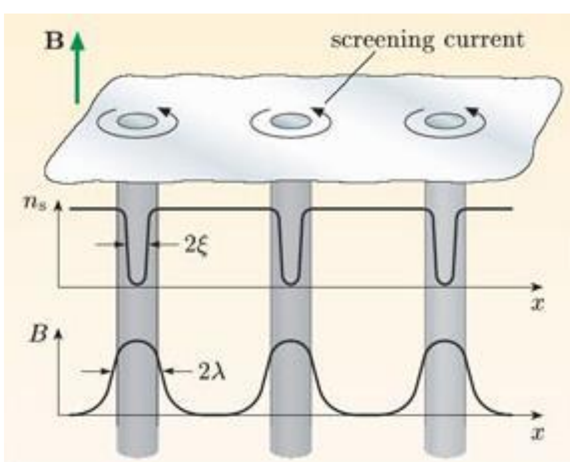
We define **coherence length** $-\frac{\boldsymbol{h^2}}{\boldsymbol{2ma}} = \boldsymbol{\xi^2(T)}$ which represents the length scale on which normalised order parameter varies from 0 to 1.

We also define **penetration depth** which is equivalent to London theory of superconductivity $\lambda(T) = \sqrt{\frac{mc^2}{16\pi\, e^2\psi_0^2}}$.



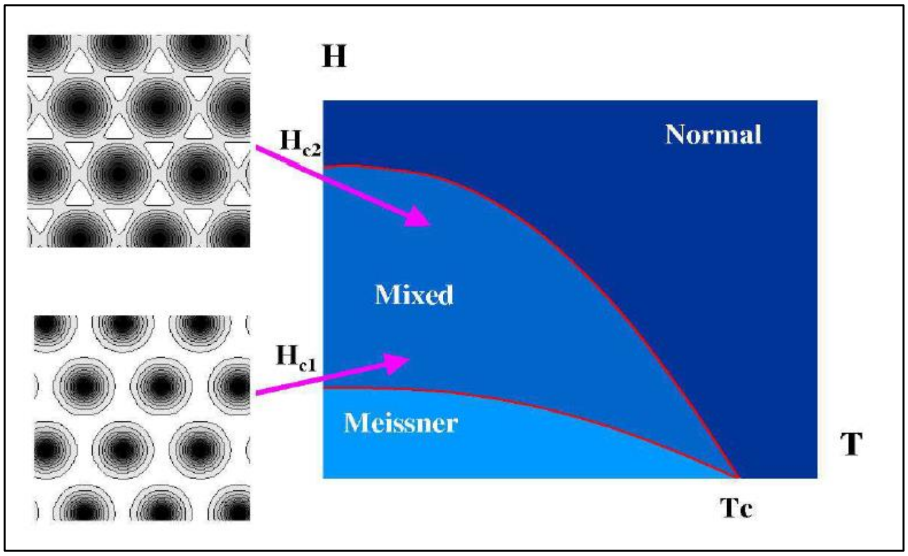
This was the case for time independent GL theory. Now we proceed to introduce **TDGL**, especially for type II SC.

Below a certain field, we still have a perfect diamagnet and no long range order for the electrons. In fields above H_{c_1} the magnetic flux penetrates the material. The flux is carried by the vortices



Order parameter goes to 0 at the centre of flux.

with parameters described above. Vortices can move during saturation as a result of interaction with other vortices and a transport current. It gives rise to an electric field, therefore resistivity. Many studies base on making the vortices immobile. In type II SC, where the vortex degree of freedom is not negligible, the normal state is separated by those H_{c_1} and H_{c_2} $where$ $they$ $divide$ $to \sim \kappa^2$. Typical solution for us is between those two field barriers. Magnetic fields constrained to vortices overlap, giving us nearly homogeneous superposition. The behaviour of so called Abrikosov vortices is described by the figure below.



The equations for TDGL theory generalised by Schmidt, which give us the dynamics of vortex in SC read as:

$$\frac{h}{2mD}\left(\frac{\partial}{\partial t}+\frac{iq}{h}\Phi\right)\psi=-\frac{1}{2m}\left(\frac{h}{i}\nabla-qA\right)^2\psi+\alpha(T)\psi-\beta|\psi|^2\psi$$

$$\sigma\left(\frac{\partial A}{\partial t}+\nabla\phi\right)=\frac{qh}{2mi}(\psi^*\nabla\psi-\psi\nabla\psi^*)-\frac{q^2}{m}|\psi|^2A-\frac{1}{\mu_0}\nabla x(\nabla xA-H)$$

Where ϕ is a scalar potential, and α, β, D are material parameters.

The most general boundary conditions consist of:

$$\left(\frac{h}{i}\nabla\psi-qA\psi\right)\cdot n=0$$

$$\nabla xA=H$$

$$\left(\frac{\partial A}{\partial t}+\nabla\phi\right)\cdot n=0$$

After that, as before, we can put a simple gauge transformation to a function. The theory consists of more information, but for the case of this paper those won't be mentioned. The theory itself is further improved by considering topological symmetry in the superconductors and its' impact on vortices creation

2. COMSOL SIMULATION AND GEOMETRY

The simulation was based on the paper published by Tobias Bonsen [1]. Having the time dependent Ginzburg-Landau equations (using $\hbar = c = e = 1$ units):

$$\frac{d\psi}{dt} = -\left(\frac{i}{\kappa}\nabla + \boldsymbol{A}\right)^2 \psi + \psi - |\psi|^2\psi$$
$$\sigma\frac{d\boldsymbol{A}}{dt} = \frac{1}{2i\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) - |\psi|^2\boldsymbol{A} - \nabla\times\nabla\times\boldsymbol{A}$$

One has to rewrite those equations to use them in COMSOL. Therefore we define

$$\psi = u_1 + iu_2$$
$$\boldsymbol{A} = \begin{bmatrix} u_3 \\ u_4 \end{bmatrix}$$

So the G-L equations take the form:

$$\frac{du_1}{dt} = \frac{1}{\kappa^2}\Delta u_1 + \frac{2}{\kappa}\left(u_3u_{2,x} + u_4u_{2,y}\right) + \frac{1}{\kappa}\left(u_{3,x} + u_{4,y}\right)u_2 - (u_3^2 + u_4^2)u_1 - u_1 - (u_1^2 + u_2^2)u_1$$
$$\frac{du_2}{dt} = \frac{1}{\kappa^2}\Delta u_2 - \frac{2}{\kappa}\left(u_3u_{1,x} + u_4u_{1,y}\right) - \frac{1}{\kappa}\left(u_{3,x} + u_{4,y}\right)u_1 - (u_3^2 + u_4^2)u_2 - u_2 - (u_1^2 + u_2^2)u_2$$
$$\sigma\frac{du_3}{dt} = \frac{1}{\kappa}\left(u_1u_{2,x} - u_2u_{1x}\right) - (u_1^2 + u_2^2)u_3 + \frac{d}{dx}\left(u_{4,x} - u_{3,x}\right) - B_a$$
$$\sigma\frac{du_4}{dt} = \frac{1}{\kappa}\left(u_1u_{2,x} - u_2u_{1,x}\right) - (u_1^2 + u_2^2)u_4 + \frac{d}{dy}\left(-u_{4,x} + u_{3,y}\right) + B_a$$

Where we assumed the boundary conditions:

$$\nabla\psi\cdot\boldsymbol{n} = 0$$
$$\nabla\times\boldsymbol{A} = \boldsymbol{B_a}$$
$$\boldsymbol{A}\cdot\boldsymbol{n} = \boldsymbol{0}$$

Which can be simplified defining another variable u_5:

$$\nabla\cdot\begin{pmatrix} u_3 \\ u_4 \end{pmatrix} = u_{3,x} + u_{4,y} + u_5$$

Using the general form of a PDE (seen below)

$$\boldsymbol{e_a}\frac{d^2\boldsymbol{u}}{dt^2} + \boldsymbol{d_a}\frac{d\boldsymbol{u}}{dt} + \nabla\cdot\boldsymbol{\Gamma} = \boldsymbol{F}$$

One can write the coefficients as:

$$
\mathbf{d}_a = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \sigma & 0 & 0 \\ 0 & 0 & 0 & \sigma & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix},
$$

$$
\mathbf{\Gamma} = \begin{bmatrix} [-u_{1,x}/\kappa^2, -u_{1,y}/\kappa^2]^T \\ [-u_{2,x}/\kappa^2, -u_{2,y}/\kappa^2]^T \\ [0, u_{4,x} - u_{3,y} - B_a]^T \\ [-u_{4,x} + u_{3,y} + B_a, 0]^T \\ [u_3, u_4]^T \end{bmatrix},
$$

$$
\mathbf{F} = \begin{bmatrix} 2(u_3 u_{2,x} + u_4 u_{2,y})/\kappa + (u_{3,x} + u_{4,y})u_2/\kappa - (u_3^2 + u_4^2)u_1 + u_1 - (u_1^2 + u_2^2)u_1 \\ -2(u_3 u_{1,x} + u_4 u_{1,y})/\kappa - (u_{3,x} + u_{4,y})u_1/\kappa - (u_3^2 + u_4^2)u_2 + u_2 - (u_1^2 + u_2^2)u_2 \\ (u_1 u_{2,x} - u_2 u_{1,x})/\kappa - (u_1^2 + u_2^2)u_3 \\ (u_1 u_{2,y} - u_2 u_{1,y})/\kappa - (u_1^2 + u_2^2)u_4 \\ u_{3,x} + u_{4,y} + u_5 \end{bmatrix}.
$$

Additionally we assume the boundary condition $-\boldsymbol{n} \cdot \boldsymbol{\Gamma} = 0$, which means that the superconducting current is parallel to the Edge of the sample.

The external magnetic field is taken in the z-direction. Because of gauge invariance for the magnetic vector potential, one can use the symmetric gauge defined as:

$$
\boldsymbol{A} = [-0.5B_a y, 0.5B_a x, 0]
$$

The simulations were made for different magnetic field strengths, various G-L parameters κ and conductivities σ. The influence of both magnetic field and G-L parameters are considered in the analysis.

The Energy of the system is calculated for selected parameters using the formula:

$$
E_{total} = E_{cond} + E_{mag} + E_{int}
$$

$$
E_{cond} = \int_\Omega d\Omega \left(\frac{1}{\kappa^2} |\nabla\psi|^2 - |\psi|^2 + \frac{1}{2}|\psi|^4 \right) \quad - \quad \textit{condensation energy of the system}
$$

$$
E_{int} = \int_\Omega d\Omega \left[\mathrm{Re}\left(\frac{i}{\kappa} \boldsymbol{A}(\psi^* \nabla\psi - \psi\nabla\psi^*) \right) + |\boldsymbol{A}|^2 |\psi|^2 \right] \quad - \quad \textit{interaction of the system}
$$

$$
E_{mag} = \int_\Omega d\Omega (|\boldsymbol{B_a} - \nabla \times \boldsymbol{A}|^2) \quad - \quad \textit{magnetic energy of the system}
$$

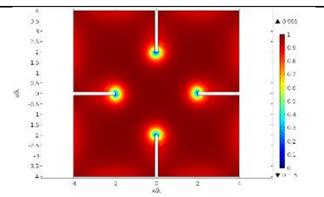
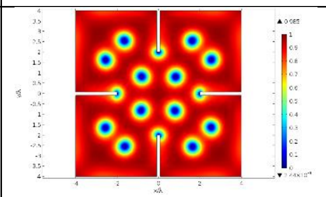
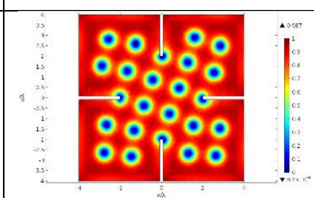
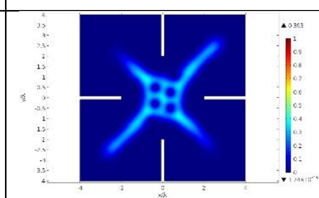
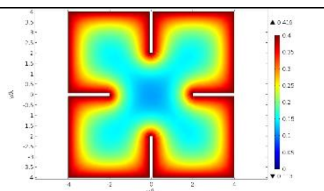
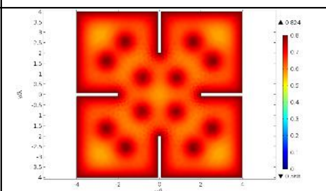
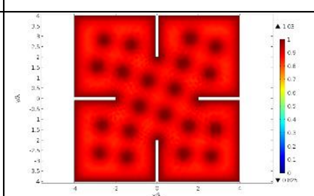
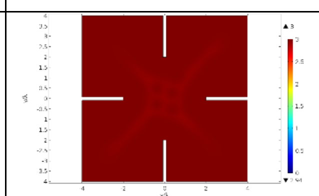
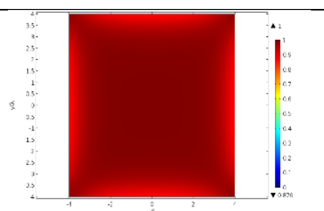
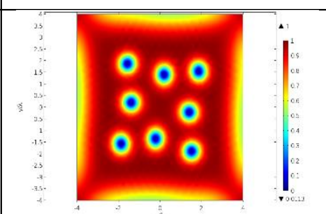
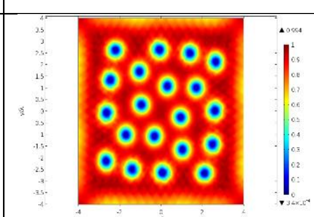
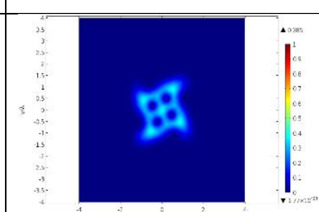
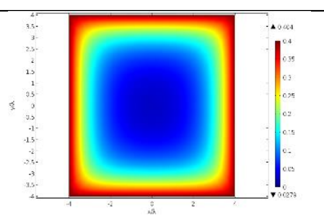
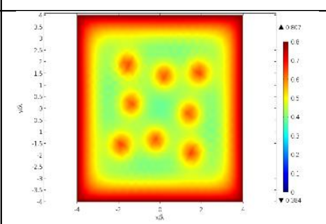
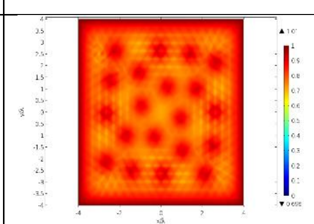
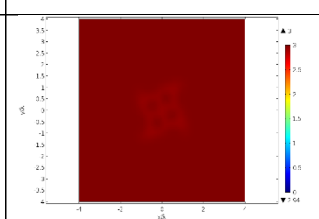
Analysis of the Energy graph one can see when the vortices nucleate.

3. ANALYSING RESULT

3.1. Square superconductor

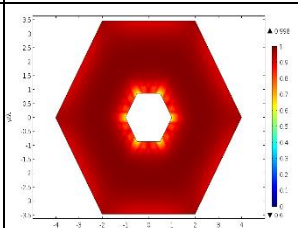
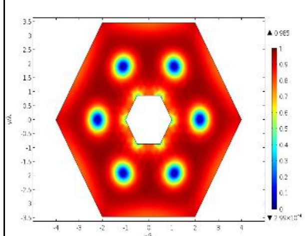
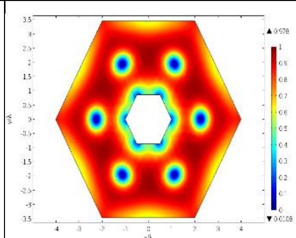
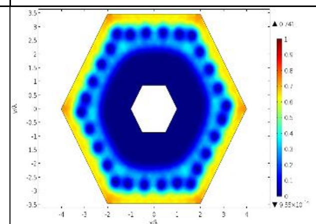
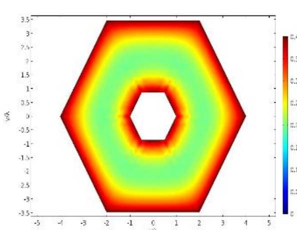
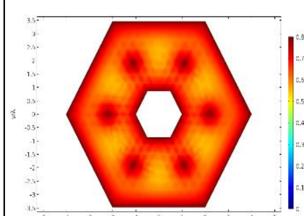
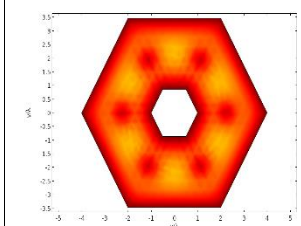
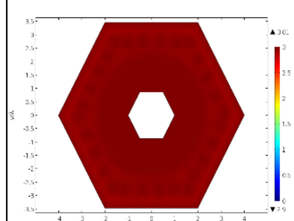
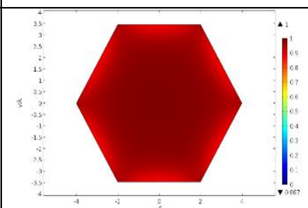
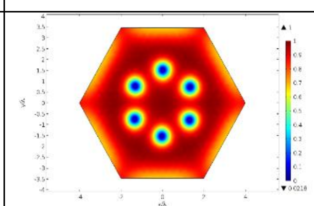
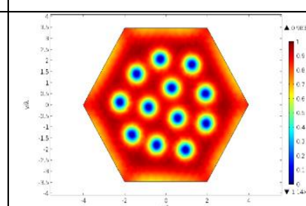
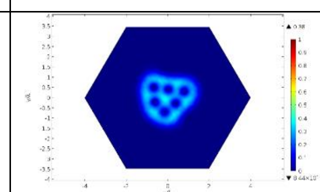
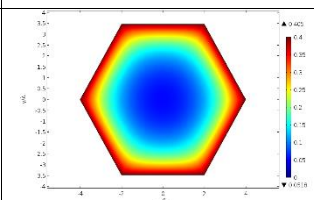
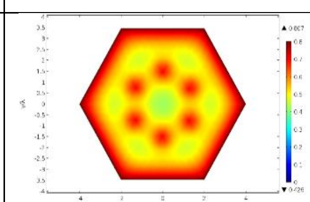
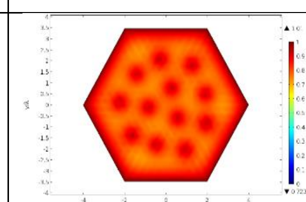
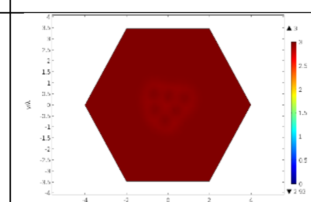
In this section we investigate the square geometry for different external magnetic fields. First we last the system till the Energy starts to stabilizes and investigate the influence of the magnetic field. Then we analyse the nucleation of vortices for selected parameters. The table (Tab.3.1) shows the change of the order parameter $|\psi|$ and the magnetic field in the sample B for external magnetic fields. One could note, that for $B_a = 3$ the order parameter starts to vanish. That's because the field is closing up to the critical field B_{c2}, which defines the transition to the normal state. In contrast to the field $B_a = 0.4$, where the superconductor is in the Meissner phase. Below the critical field B_{c1} the vorticies can't nucleate at any time.

(Tab.3.1) Magnetic field dependence of the order parameter

Magnetic field	B_a	0.4	0.8	1	3
Defected SC	$\|\psi\|^2$				
	B				
Non-defected SC	$\|\psi\|^2$				
	B				

3.2. Hexagonal superconductor

In analogy to the earlier case we choose the same parameters for this geometry. The procedure is exactly the same. The same as for the square geometry occurs for the hexagonal superconductor. We can distinguish each phase by the order parameter. In the Meissner phase it is uniform in the sample (except the boundaries, where we have fluctuations) and equals $|\psi| = 1$. The table (Tab. 3.2) presents the order parameter and the field in the sample in each case of the external magnetic field:

(Tab.3.2) Magnetic field dependence of the order parameter					
Magnetic field	B_a	0.4	0.8	1	3
Defected SC	$\lvert\psi\rvert^2$				
	B				
Non-defected SC	$\lvert\psi\rvert^2$				
	B				

As expected the last case presents the external field almost entirely penetrating the sample, which means (in comparison with the order parameter) that we are close the transition point to the normal state.

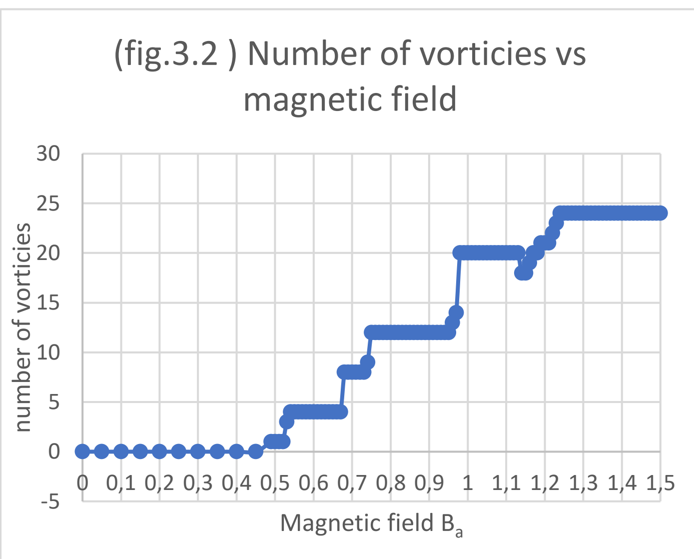
3.3. Vortices counting

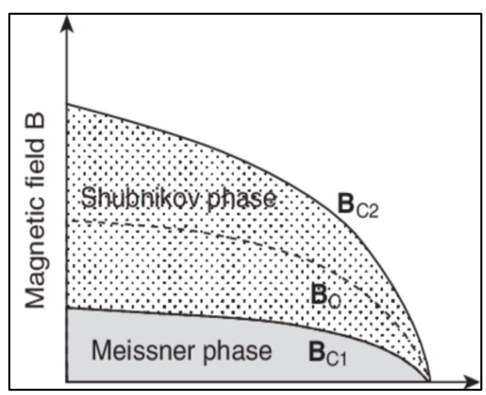
3.3.1. External field

An important aspect of simulating a type II superconductor is to know the critical fields for one. The Shubnikov phase lies between two critical fields, which where numerically found in this subsection. The phase diagram for a type II superconductor is shown in (fig. 3.1). One can count the number of vortices for a given field, which is done in the figure (fig.3.2). One can note the lower critical field between the Meissner phase and the Shubnikov phase $B_a = 0{,}49$. We also conclude that the number of vortices is much higher for higher fields. For fields larger than $B_a = 1{,}5$ the vortices start to combine as there isn't enough space for them to stay apart [2]. Above a field around $B_a = 2{,}55 - 2{,}6$ the order parameter vanishes on the boarder and stays only nonzero in the middle of the sample. This yields that in fields higher than $B_a = 2.7$ the sample is in the normal state.

3.3.2. Time nucleation

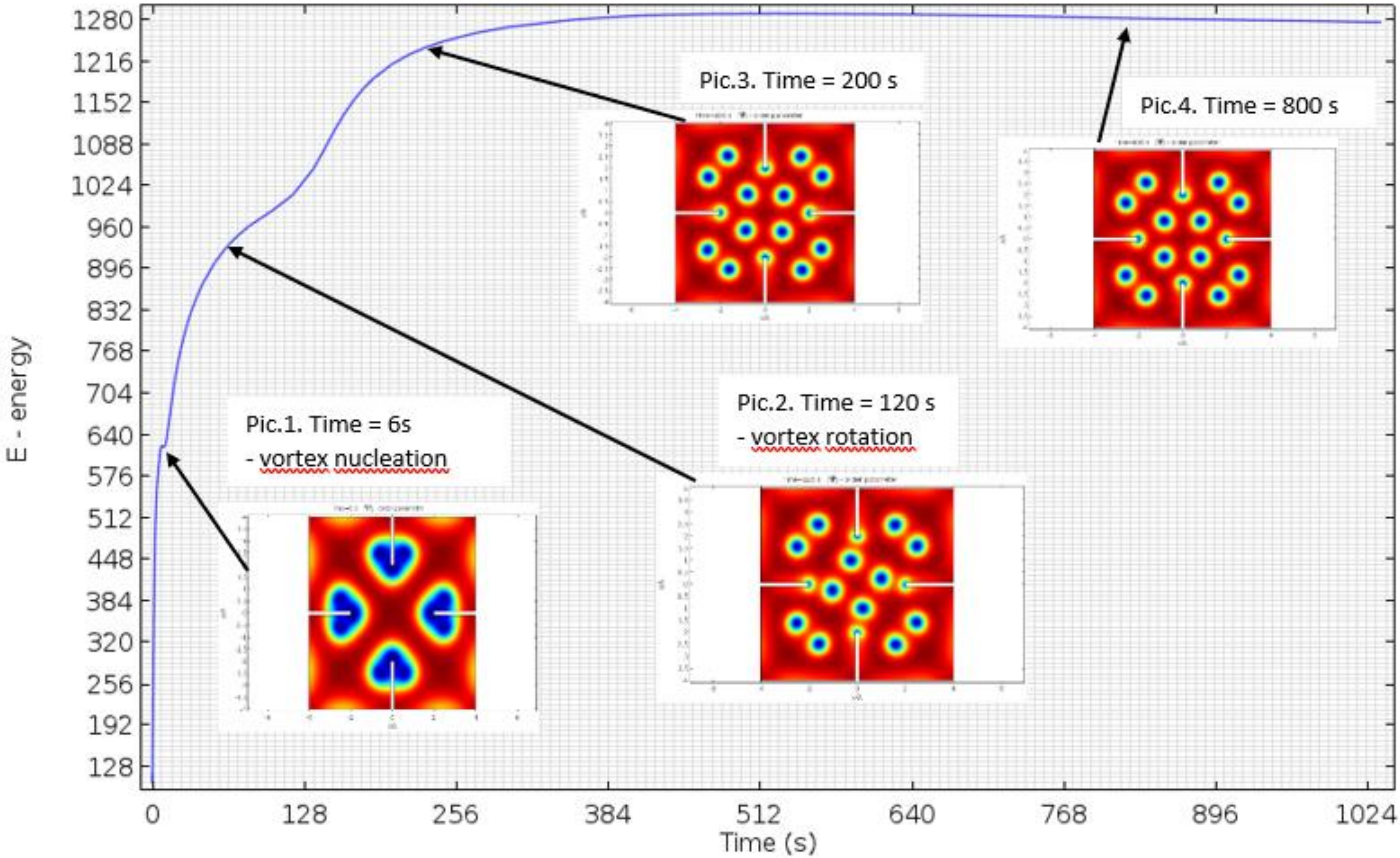
Here we investigate the generation and movement of the vortexes over time for the defected square geometry. One can note that the vortices stabilize in a square lattice. For the other geometries we can see the triangular lattice for the vortexes. Looking at the overall Energy of the system across the timelapse one can note when the vortices are nucleated and what happens later. The origin of the nucleated vorticies is always the distortion (indentation etc.) The simulation was last for 1000 timesteps. The first vortices nucleated in the 6 second (pic.1), then around the 120 second the lattice started to relocate (pic.2) to find its steady-state (pic.3-4). And finally the system is at a steady-state, which corresponds to the last plot in (fig.3.3)





(fig.3.1) Type II superconductor phase diagram

(fig.3.3) Energy of the system



4. FINAL REMARKS

To summarize one can note that each case is characterized by the same unchanged parameters. For instance in each plot we see some small fluctuations on the boundaries which are associated with the London penetration depth λ which was kept constant the G-L parameter was kept constant, but $\kappa = \lambda/\xi$). Th elondon penetration depth gives us information about how much does the field intrude in the sample. On the othe hand we see something similar in the order parameter. The fluctuations on the boundary are here associated by the coherence length.

Most of the Times the Abrikosov lattice is shown to be triangular (or hexagonal). Only in special cases one can see different lattices, for example the square lattice in the middle in the for the square superconductor with slits. If we had analysed a cylindrical geometry one would expect vortices lining on a circle [4].

The simulations in this paper presents the instability of the Shubnikov phase for high magnetic fields. An important fact is that the vortex sources are always the sharp edges [3] in the system. For the square geometry the vortexes nucleate from the slits (for high field above 1.1 they nucleate from the side too) . For the hexagon lattice the vortices originate from the sharp edges of the inside hexagon. This result is rather unphysical, because it takes a relative high vortex to enter the material. One possible solution could be to refine the mesh [1], but it turns out the mesh convergence of this problem is very slow.

Comparing geometries with defects (slits, holes etc) to ones without one can immediately notice that the disturbed superconductor is more resistant to the magnetic field maintaining a non-zero order parameter. This could be caused by the discontinuity of $\frac{d\psi}{dx}$ on sharp edges [4]. This yields one could use distortion to maintain a penetrating high magnetic field in the superconductor giving high application possibilities. For instance in newest magnetic resonance devices or SQUID (Superconducting Quantum Interference Device).

5. REFERENCES

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