Screw dislocations in a mesoscopic Smectic A liquid crystal phase

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Amos Schtalheim

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Dedicated with love to my father Dr. Alexander Schtalheim who is an inspiration to me. Without the support of my parents I would not have come this far.
With admiration to my wife Moiken who has given me the strength and wisdom to manage difficult times, without her support and love I doubt that I would have succeeded.

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Abstract

This thesis derives analytically and calculates the existence and appearance of screw dislocations in a mesoscopic smectic A liquid crystal sample.

Screw dislocations have first been observed experimentally by Goodby et al (1989), a short time after Renn and Lubensky (1988) published their theoretical work describing the twist grain boundary phase, which involves such screw dislocations and is analogous to the Abrikosov vortex phase.

The theoretical basis of this work is the de Gennes analogy (1972) between the free energies of superconductors and the smectic A phases. This analogy enabled to implement the Bogomol'nyi method, for flat two-dimensional infinite superconductors at the dual point, on infinite long cylindrical smectic A samples lying in an external twist field, which is parallel to the cylinder axis. For such systems the minimization of the energy is topological. Moreover, for a cylinder of finite mesoscopic radius it is possible to obtain an expression for the energy which includes the number of the screw dislocations. This enables to determine the exact number of the screw dislocations in equilibrium as a function of the applied external twist field.

The value of the external field needed for the entrance of the first dislocation is calculated for a specific set of system parameter values and presented in a matching figure. It is also shown that the result obtained is valid for a finite area of parameter values.

Glossary

General

Ψ-Complex order parameter
φ-Phase of the order parameter
ψ_0-Equilibrium value of the order parameter
ψ-Dimensionless order parameter
F-Free energy
f-Free energy density
T-Temperature
V-Volume
Ω-Surface
Γ-Contour

Superconductors

$\boldsymbol{j}$-Current density
λ-Mean field penetration depth
ξ-Coherence length
κ-Ginzburg parameter
f_s-Superconductor free energy density
f_n-Normal phase free energy density
$\boldsymbol{B}$-Magnetic flux density
B_c-Critical magnetic flux density
$\boldsymbol{A}$-Vector potential
ϕ-Magnetic flux
ϕ_0-Quantum fluxoid
α, β-Landau mean field energy parameters
e-Electron charge
c-Speed of light
$\hbar$-(Planck constant)$/(2\pi)$

m-Mass
n-Number of vortices (integer)
σ-Surface energy

Liquid crystals

F_{SmA}-SmA free energy
$F_{nematic}$-Nematic free energy
$G_{cholesteric}$-Cholesteric Gibbs free energy
r, g-Landau mean field energy parameters
λ_T-Twist mean field penetration depth
$\xi_\perp$-Perpendicular coherence length
$C_\perp$-de Gennes SmA perpendicular energy parameter
$C_{||}$-de Gennes SmA parallel energy parameter
K_1, K_2, K_3-The Frank Oseen splay, twist and bend energy parameters
$\boldsymbol{h}$-Chiral field
$\boldsymbol{P}$-Pitch
l_p-Pitch length
k_0-Wave number of the cholesteric field
ρ-Density
q_s-SmA density wave number
φ-Phase of the SmA density
$\boldsymbol{N}$-SmA layer direction
$\boldsymbol{n}$-Director
$\delta\boldsymbol{n}_\perp$-Projection of a slightly tilted director on the perpendicular direction to the director's direction
$\boldsymbol{\nabla}_\perp$-Two dimensional nabla that lies in the perpendicular direction to the director's direction
u-SmA layer displacement
$\boldsymbol{\tau}$-Twist flux density
Φ_{SmA}-Twist flux through a SmA sample
Φ_{LP}-Little Parks twist flux
δ-Penetration depth of a finite size sample
R-Sample radius
l-Number of screw dislocations (integer)

Chapter 1

Introduction

The transition of a *nematic* to a *smectic A* phase in liquid crystals is in many properties similar to the transition of a normal metal to the superconducting phase. This similarity was first pointed out by de Gennes back in 1972, when he proposed to describe the *smectic A* phase by a complex scalar order parameter like Landau and Ginzburg did 20 years before in their phenomenological theory for superconductors. This enabled de Gennes to present a thermodynamic equation that describes the *smectic A* to *nematic* phase transition by considering their relevant free energies. In this thesis this analogy was used to further develop the understanding of liquid crystals.

In 1988 Renn and Lubensky showed that this analogy can be expanded. They found an analogous phase to the Abrikosov phase in superconductors. It is the "Twist Grain Boundary Phase " (*TGB*). Soon after experimental evidence for the existence of the *TGB* phase followed. In their work Renn and Lubensky showed that the *TGB* phase is an energetically stable phase that includes topological defects inside a sample. They found that it lays between the *smectic A* and the *cholesteric* phases. This is in perfect analogy to superconductors of the second kind; when inserted in a strong magnetic field it leads to the creation of vortices in the sample. The *cholesteric* phase can be compared to a normal metal that is exposed to a magnetic flux. The *smectic A* is then the equivalent to the Meissner phase.

However, the reason for the existence and creation of vortices in superconductors was not clear until E.Akkermans and K.Mallick showed (1999) that they can be analytically derived from the Ginzburg-Landau free energy. This could be derived for very small (mesoscopic) disclike superconductor samples at a special integrable point. The question addressed in this thesis is whether it is possible to do a similar analytical derivation to show the existence of topological defects in *smectic A* samples from the de Gennes free energy. For that purpose we shall try to follow the footsteps of E.Akkermans

and K.Mallick while applying it to liquid crystals.

1.1   Introduction to superconductivity

Superconductors can be described phenomenologically by the Ginzburg-Landau equations (1950). It is a macroscopic description of a phenomena which is in essence a quantum phenomena and thus can describe very easily quantum macroscopic effects. Landau and Ginzburg figured out that the transition to superconductivity is a second-order transition and thus described it in the framework of Landau's "mean field theory". This theory is based on the assumption that the phase transition to a superconductor involves a transition to a more ordered phase. In order to describe this transition they defined a complex order parameter $\Psi = |\Psi|e^{i\varphi}$. If $\Psi \neq 0$ it points out the existence of a superconducting phase. It is then possible to write a mean field expression:

$$f_s = f_n + \alpha|\Psi|^2 + \frac{\beta}{2}|\Psi|^4. \tag{1.1}$$

Since Ψ is complex, whereas the energy must remain real, f_s is expanded in powers of $|\Psi|$. Furthermore a second order type transition forces even powers. In contrast, for $\Psi = 0$ the phase is normal. The equilibrium energy must be finite, therefore at least one extra term in fourth power has to be added. The equilibrium value of Ψ is attained by minimizing the free energy. The phase transition is a function of the temperature. This property is included by defining $\alpha \propto (T - T_c)$ at the vicinity of the transition temperature T_c. It is also assumed that β is positive and independent of the temperature at T_c. As a result when $T > T_c \Rightarrow \alpha > 0$, the minimization of f_s with respect to Ψ yields $\Psi = 0$ which means that the phase is normal. On the other hand for $T \leq T_c$ the minimization of f_s leads to $|\Psi|^2 = \psi_0^2 = -\frac{\alpha}{\beta} \geq 0$. As the temperature decreases below the critical temperature, the order parameter varies continuously from 0 to a positive finite value. When a magnetic field is introduced, its energy must be added to the free energy in the following way:

$$f_s = f_n + \alpha|\Psi|^2 + \frac{\beta}{2}|\Psi|^4 + \frac{B^2}{8\pi}. \tag{1.2}$$

If the equilibrium value of $|\Psi|$ is substituted into (1.2), it leads to $f_s - f_n = \frac{-\alpha^2}{2\beta} + \frac{B^2}{8\pi}$. It is therefore understood that the critical magnetic field corresponds to $\frac{-\alpha^2}{2\beta} = \frac{-B_c^2}{8\pi}$. The contribution to the energy due to spatial variation of the magnitude of the order parameter is also considered. It is

also introduced in even powers.

$$f_s = f_n + \alpha|\Psi|^2 + \frac{\beta}{2}|\Psi|^4 + \frac{\hbar^2}{2m^*}|\nabla\Psi|^2 + \frac{B^2}{8\pi} \qquad (1.3)$$

The order parameter is therefore spatially dependent $\Psi \to \Psi(r)$. Still equation (1.3) does not describe one very important property of superconductors. It is the Meissner effect, which states that the magnetic field in a superconductor ceases to be a thermodynamic variable. Instead, it is determined by the system parameters in order to minimize its energy. In fact, the lowest energy is obtained when the order parameter phase is such that it expels the magnetic field completely from the superconductor. The Meissner effect is included by introducing the magnetic vector potential into the equation. However, since the free energy is a real quantity it is also necessary to keep it gauge invariant. This is exactly the reason why the order parameter is a complex quantity. The fourth term in the energy expression is therefore changed to $\frac{1}{2m^*}(\hbar\nabla\varphi - \frac{e^*\boldsymbol{A}}{c})^2|\Psi|^2$, where φ is the phase of the order parameter. It will be shown that the gradient of this phase is connected to the existence of supercurrents in the sample. This term is inserted to the free energy combined with the gradient term of the magnitude of Ψ, resulting in the general compact form of all gauge invariant theories. Finally the Ginzburg-Landau free energy is:

$$f_s = f_n + \alpha|\Psi|^2 + \frac{\beta}{2}|\Psi|^4 + \frac{1}{2m^*}\left|\left[-i\hbar\nabla - \frac{e^*\boldsymbol{A}}{c}\right]\Psi\right|^2 + \frac{B^2}{8\pi}. \qquad (1.4)$$

The star sign over the electron charge stands for 'effective'. At the time, Landau and Ginzburg were not aware of superconducting pairs which according to BCS theory suggests $e^* = 2e$. However, (1.4) is more general than a theory for superconductive metals alone. It is also important to understand that m^* appearing in (1.4) is not the electron mass of inertia. The electron mass of inertia has no effect on the system. The mere word 'super' suggests that there exists no mass of inertia in the system. This parameter just sets the right gauge for the free energy, at a place where mass was the correct dimension needed. A further advantage rises from the inclusion of a mass parameter since it yields a similarity between the first Ginzburg-Landau equation and the Schrödinger equation.

1.2   The Ginzburg-Landau equations

As the free energy is defined, Ginzburg and Landau have proceeded in the conventional way to derive the physical properties of the system, which is

by using the method of variation and demanding the action to be in its extremum.

$$\delta I = \int dt \left\{ \frac{\partial \mathbf{F}}{\partial \psi} \delta \psi + \frac{\partial \mathbf{F}}{\partial \psi^*} \delta \psi^* + \frac{\partial \mathbf{F}}{\partial \mathbf{A}} \delta \mathbf{A} \right\} = 0 \tag{1.5}$$

where $\mathbf{F} = \int f dV$. Since I is to be in its extremum for every A, each of the integrand terms must be separately equal to zero. Because of the even powers of the free energy, the variation with Ψ or Ψ^* will give similar complex conjugate equations, therefore only the second term with Ψ^* is considered. It yields an equation for the order parameter

$$0 = \int dV \left[\frac{\partial f}{\partial \Psi^*} \right] \delta \Psi^* \;\; = \;\; \int dt \{ \alpha \Psi + \frac{\beta}{2} \frac{\partial}{\partial \Psi^*} (\Psi^* \Psi \Psi^* \Psi) + \tag{1.6}$$

$$+ \;\; \frac{1}{2m^*} \frac{\partial}{\partial \Psi^*} \left| \left(\frac{\hbar}{i} \nabla - \frac{e^* \mathbf{A}}{c} \right) \Psi \right|^2 + \frac{\partial}{\partial \Psi^*} \frac{(\nabla \times \mathbf{A})^2}{8\pi} \} \delta \Psi^*.$$

The complex form of the order parameter is inserted in order to calculate the derivative of the term inside the absolute sign. The last term drops and the following integral is obtained:

$$\int dV [\alpha \Psi + \beta |\Psi|^2 \Psi + \frac{1}{2m^*} (-i\hbar \nabla - \frac{e^* \mathbf{A}}{c}) \Psi (i\hbar \nabla - \frac{e^* \mathbf{A}}{c})] \delta \Psi^*. \tag{1.7}$$

The second term can be handled by means of integration by parts and then followed by using the Gauss theorem on $\nabla \delta \Psi^*$, keeping in mind that in variation calculus the variation on the boundary is zero $\delta \Psi^* \mid_{boundary} = 0$. Since the result of minimization should stand for every $\delta \Psi^*$ the integrand has to vanish. This leads to the equation for the order parameter, which is the first differential Ginzburg-Landau equation

$$\frac{1}{2m^*} (-i\hbar \nabla - \frac{e^* \mathbf{A}}{c})^2 \Psi + \alpha \Psi + \beta |\Psi|^2 \Psi = 0. \tag{1.8}$$

The similarity to the Schrödinger equation is striking. But in contrast to the latter, the Ginzburg-Landau equation includes the non linear term $\beta |\Psi|^2 \Psi$, making equation (1.8) difficult to solve.

The variation of the vector potential yields the second Ginzburg-Landau equation.

$$\begin{aligned} 0 \;\; &= \;\; \int dV \frac{\partial f}{\partial \mathbf{A}} \delta \mathbf{A} = \int dV [\frac{1}{2m^*} \frac{\partial}{\partial \mathbf{A}} |(\frac{\hbar}{i} \nabla - \frac{e^* \mathbf{A}}{c}) \Psi|^2 + \frac{\partial}{\partial \mathbf{A}} \frac{(\nabla \times \mathbf{A})^2}{8\pi}] \delta \mathbf{A} \\ &= \;\; \int dV \{ \frac{1}{2m^*} [\frac{-e^*}{c} (i\hbar \nabla) \Psi^* (-i\hbar \nabla - \frac{e^* \mathbf{A}}{c}) \Psi - \tag{1.9} \\ &- \;\; \frac{e^*}{c} (i\hbar \nabla - \frac{e^* \mathbf{A}}{c}) \Psi^* (-i\hbar \nabla) \Psi] \delta \mathbf{A} + \frac{2(\nabla \times \mathbf{A})(\nabla \times \delta \mathbf{A})}{8\pi} \}. \end{aligned}$$

The vector identity $\nabla(\mathbf{A} \cdot \mathbf{B}) = \mathbf{B}(\nabla \times \mathbf{A}) - \mathbf{A}(\nabla \times \mathbf{B})$ was used, so that the last term becomes $(\nabla \times \mathbf{A})(\nabla \times \delta\mathbf{A}) = \nabla(\delta\mathbf{A}(\nabla \times \mathbf{A})) + \delta\mathbf{A}(\nabla \times (\nabla \times \mathbf{A}))$. The method of integration by parts is followed by the use of $\nabla \times \nabla \times \mathbf{A} = \nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{j}$ and the Gauss theorem. Since the variation is zero at the boundary, inserting the boundary condition $(\frac{\hbar}{i}\nabla - \frac{e^*\mathbf{A}}{c})\Psi|_n = 0$ stating that there is no current passing the surface perpendicularly, leads to

$$0 = \int dV [\frac{\mathbf{j}}{c} + \frac{ie^*\hbar}{2m^*c}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) + \frac{2e^*}{m^*}|\Psi|^2\mathbf{A}]\delta\mathbf{A}. \tag{1.10}$$

Since (1.10) has to be valid for every arbitrary vector potential, the integrand must vanish. This leads to the second Ginzburg-Landau equation

$$\mathbf{j} = \frac{e^*\hbar}{i2m^*}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) - \frac{e^{*2}}{m^*c}|\Psi|^2\mathbf{A}. \tag{1.11}$$

Equation (1.11) reminds of the quantum probability density current expression in the present of an electromagnetic field. It seems that the current density is not gauge invariant, however a closer examination will show that the vector potential is gauged by the first term of (1.11).

Let us now examine equations (1.8) and (1.11). If a superconducting sample is placed into a weak magnetic field and $|\Psi| = \psi_0$, where ψ_0 is the order parameter value in equilibrium with no spatial variations, then (1.11) becomes

$$\nabla \times \mathbf{j}_z = \nabla \times \nabla \times \mathbf{B} = -\frac{e^{*2}}{m^*c}\psi_0^2\mathbf{B}. \tag{1.12}$$

Assuming that the sample lies in the upper infinite space ($z > 0$), a solution for (1.11) would be $B = B_0 e^{\frac{-z}{\lambda(T)}}$, which is the Meissner effect. An exponential decay of the magnetic field into the sample with a penetration depth of λ is evident. The penetration depth obliges $\lambda^{-2} = \frac{4\pi e^{*2}\psi_0^2}{m^*c^2}$. For the first Ginzburg-Landau equation (1.8), a similar analysis can be done. If there is no current nor a magnetic field, then it is possible to gauge the order parameter in a way that it becomes a real scalar, so (1.8) becomes [12]

$$\frac{-\hbar^2}{2m}\frac{d^2|\Psi|}{dx^2} + \alpha|\Psi| + \beta|\Psi|^3 = 0. \tag{1.13}$$

It is of interest to see how the order parameter $|\Psi(x)|$ changes in the vicinity of some spatial point. For that purpose it is expressed in the dimensions of its equilibrium value, $\Psi = \psi_0\psi$. The following length scale is defined $\xi^2(T) = \frac{\hbar^2}{2m^*|\alpha|}$, so that

$$-\xi^2(T)\frac{d^2|\psi|}{dx^2} - |\psi| + |\psi|^3 = 0. \tag{1.14}$$

From the above derivation, the equilibrium value of the order parameter $\psi_0^2 = -\frac{\alpha}{\beta} \geq 0$ was used. The length over which f changes is therefore $\xi(T)$. This is the 'coherence length'.

When the equilibrium value of $|\Psi|$ is inserted into the 'penetration depth' term, it is clear that its temperature dependence, which is contained in the α parameter, is the same as for ξ. This suggests that it is of interest to define the ratio between those two characteristic lengths of the material

$$\kappa = \frac{\lambda}{\xi}. \tag{1.15}$$

This is the Ginzburg parameter. Its value at the vicinity of T_c is a constant. It depends on the inherent properties of the material from which the superconductor is made of.

1.3 Type II superconductors and the Abrikosov phase

Let us calculate the energy of a domain wall separating a superconductor from a normal material [1] for a one dimensional setup like it was used above. In this case the boundary conditions would be

$$\begin{array}{lll} |\psi| = 0 & and & B = \frac{1}{\sqrt{2}} & as & z \to -\infty \\ |\psi| = 1 & and & B = 0 & as & z \to +\infty, \end{array} \tag{1.16}$$

where $B = \frac{1}{\sqrt{2}}$ corresponds to the critical magnetic field $B = B_c$ in dimensionless units. For a gauge which sets ψ to be real, equations (1.8) and (1.11) become (1.14) and (1.12) respectively. If (1.14) is multiplied with $\frac{d|\psi|}{dz}$ and integrated, then applying the above boundary conditions yields

$$\xi^2(T)\frac{d^2|\psi|}{dx^2} = \frac{1}{2}(1 - |\psi|^2)^2. \tag{1.17}$$

Then for a material in which the Ginzburg parameter is smaller then unity $\kappa \ll 1$ (meaning $\lambda \ll \xi$), the following stands

$$\frac{d|\psi|}{dx} = \frac{\kappa}{\sqrt{2}}(1 - |\psi|^2). \tag{1.18}$$

The normalized order parameter obtained from (1.18) is $|\psi| = \tanh(\frac{\kappa z}{\sqrt{2}})$. The surface energy is given by the difference in energy between the superconducting state and the external magnetic field energy, which is calculated

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in the following way:

$$\sigma_{ns} = \frac{B_c^2}{4\pi} \int [(B - B_c)^2 - \frac{1}{2}|\psi|^4]dV. \qquad (1.19)$$

For the magnetic field values $B = 0$, $B_c = \frac{1}{\sqrt{2}}$ and the expression obtained for f it becomes:

$$\sigma_{ns} = \frac{B_c^2}{8\pi} \int_0^\infty [1 - \tanh^4(\frac{z\kappa}{\sqrt{2}})]dz. \qquad (1.20)$$

The domain wall energy is dependent on κ. For $\kappa < \frac{1}{\sqrt{2}}$ it is positive, meaning that there is a boundary separation between the phases. But, for the value $\kappa = \frac{1}{\sqrt{2}}$ the boundary energy vanishes and for $\kappa > \frac{1}{\sqrt{2}}$ it becomes negative. The meaning of a negative boundary energy is that the system would tend to create many subdivisions of the bulk into subregions in order to decrease the total energy. Magnetic flux is now allowed to pass through the divided material.

Materials with $\kappa > \frac{1}{\sqrt{2}}$ are known to be type II superconductors. A 'mixed state' is created when an external magnetic field is introduced. The order parameter is mixed with the magnetic field, so that Meissner does not apply. The value of the magnetic field inside the sample is calculated by averaging the density of all flux lines passing through the sample.

The quantization of the magnetic flux that passes through the superconductor is another important feature appearing. To show it, $\Psi = |\Psi|e^{i\varphi}$ is inserted into (1.11)and we obtain

$$j = \frac{2e\hbar}{m}|\Psi|^2(\nabla\varphi - \frac{2e}{\hbar c}\mathbf{A}) \qquad (1.21)$$

For simplicity as of now $e^* \to 2e$ and $m^* \to m$ shall be used. It is observed that a connection between the gradient of the phase and the supercurrent exists. If a hollow cylinder whose walls are thicker than the penetration depth is considered, then $|\Psi|^2 \to \psi_0^2 = const.$ and $j \to 0$ in the bulk region. An integration around a closed loop inside the bulk is possible and we can write:

$$0 = \oint \frac{j}{|\Psi|^2} = \frac{2e\hbar}{m}[\oint \nabla\varphi d\mathbf{l} - \frac{2e}{\hbar c} \oint \mathbf{A}d\mathbf{l}]. \qquad (1.22)$$

The first integral is a loop integral over the the gradient of the phase. It does not have to be zero since the phase is not a measurable physical quantity. However, the order parameter is demanded to be single valued for a 2π circulation, so that the phase of the order parameter is allowed to change in rates of $2\pi n$.

On the other hand, the second integral is

$$\frac{2e}{\hbar c}\oint \mathbf{A}d\mathbf{l} = \frac{2e}{\hbar c}\int \nabla \times \mathbf{A}d\mathbf{S} = \frac{2e}{\hbar c}\int \mathbf{B}d\mathbf{S} = \frac{2e}{\hbar c}\phi = 2\pi\frac{\phi}{\phi_0}, \qquad (1.23)$$

where $\phi_0 = \frac{hc}{2e}$ is defined to be the quantum fluxoid, it is the 'London fluxoid'. The total flux is quantized in multiples of single fluxoids

$$\phi = n\phi_0 \qquad (1.24)$$

with n being an integer. n is named 'winding number', its value will determine the amount of 'vorticity' in the system. The reason why it is called 'vorticity' will be clarified.

An important property of superconductivity is the breakdown of phase symmetry. This can be understood if the Ginzburg-Landau free energy (1.4) is examined. In a bulk in which $|\Psi|$ is constant, the term involving the gradient of $|\Psi|$ is in even powers and therefore at the minimum of the free energy it should vanish. If the complex form of Ψ is inserted, it yields $0 = \frac{1}{2m^*}(\hbar\nabla\varphi - \frac{2e\mathbf{A}}{c})^2|\Psi|^2$, so that $\nabla\varphi = \frac{2e\mathbf{A}}{\hbar c} = 2\pi\frac{\mathbf{A}}{\phi_0}$. This determines φ up to a constant. A certain potential drives a constant change in the phase of the order parameter and therefore breaks the symmetry. If the gradient is not zero a supercurrent exists. However, current exists only up to the distance of the penetration depth λ. Beyond that, the magnetic field is depressed strongly.

In order to keep a non zero magnetic field in coexistence with the order parameter in a type II superconductor, singular points of the order parameter field $\Psi \to 0$ within the bulk have to exist. Then a magnetic flux can exist. This flux is quantized. This surprising observation was done first by Abrikosov [Nobel prize 2003].

Around each such singularity there is a radius of ξ in which the order parameter changes from zero to its equilibrium value and supercurrents flow in proportion to the amount of the magnetic flux going through the singularity. This is the reason that n is the 'vorticity' of the system. Abrikosov also calculated that it is energetically preferred, in an infinite sample (because the magnetic field should be homogeneously distributed), that the flux should be spread as much as possible, so that at every singular point the flux passing through it be only one quantum flux. This is preferred to concentrating the same amount of quantized flux at one singular point. It is due to the repulsion between the supercurrents. They should therefore also distribute as distant as possible from each other. The appropriate distribution was found to be a triangular lattice. This lattice/phase that appears in type II superconductors is called the Abrikosov phase.

To summarize it, a type II superconductor in its mixed state is a triangular lattice of singular points through which quantized magnetic flux lines pass, enabling the coexistence of a mean magnetic field and the superconducting order parameter.

1.4 A short review of the liquid crystal phases

Liquid crystals are systems which exhibit short range correlations in some directions and long range order in other directions and have symmetries intermediate between those of liquids and the crystals. Liquid crystals are composed of anisotropic molecules, which can be modeled as rigid rods or ellipsoids of revolution with lengths l greater than their widths a. Their orientational order is caused mostly by repulsive interactions. At high temperature the axes of the molecules are randomly oriented as well as their center of mass. This is the *isomorphic* phase [8].
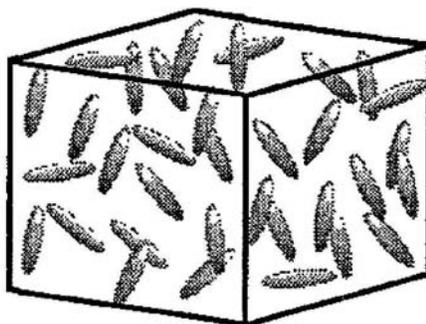
Figure 1.1: Isomorphic Phase: This phase is characterized by molecules whose interaction energy is much weaker than their thermal energy. Thus no particular order is established, it is practically a normal liquid.

Nematic: As the temperature sinks, the first condensed phase which arises is *nematic*. In that phase the molecules tend on average to have a common symmetry axis specified by a unit vector $\hat{\mathbf{n}}$ called the Frank director, as of now the 'director'. However, their center of mass stay at random so that they still compose an isotropic fluid in all directions. The *nematic* phase breaks rotational isotropy but not translational invariance [8]. In the *de Gennes* description, the *nematic* phase can be treated as the equivalent to the state of a normal metal that is not placed in an external magnetic field.
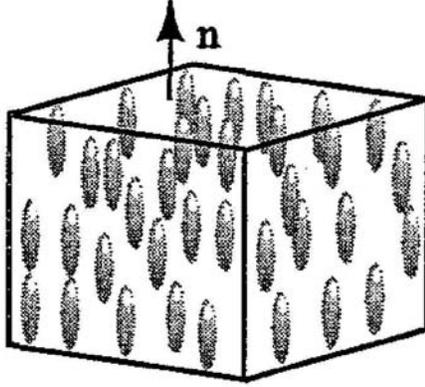
Figure 1.2: Nematic Phase: This phase is characterized by the appearance of the director. This is a unit vector in the mean direction of the molecules. The molecules in the sample deviate only slightly from this direction and are on average parallel to each other but their center of mass is still positioned arbitrarily.

Cholesteric: When chiral molecules are added to a *nematic* liquid crystal, a twisted/chiral *nematic* state results. In this state the local director rotates in a helical pattern along a specific axis. We define the pitch **p** to lie in the direction of that axis. Its size is the distance in which the director undergoes one full rotation around this axis $L_p = \frac{2\pi}{k_0}$. k_0 is the wave number of the Frank director in the *cholesteric* phase. The size of **p** depends on the concentration and degree of chirality of the chiral molecules and is typically of the order of several thousand angstroms [8]. In the description by *de Gennes*, the *cholesteric* phase can be treated as the equivalent to the state of a normal metal exposed to an external magnetic field.

Smectic A: Sometimes when the *nematic/cholesteric* is cooled, the molecules condensate to a modulated phase called the *Smectic A (SmA)* phase. In this phase the center of mass of the molecules are modulated to form a layered system. The following density equation describes it [11].

$$\rho(\mathbf{r}) = \rho_0 + \rho_1 \cos(q_s z - \varphi) + \cdots \qquad (1.25)$$

The $\hat{z}$ direction is set to be the reference axis. It is aligned to the layers direction, which is defined to be **N**. The wave number of the density modulation of the molecules is $q_s = \frac{2\pi}{d}$, where d is the distance between consecutive layers. In *SmA* the director $\hat{n}$ is parallel to the
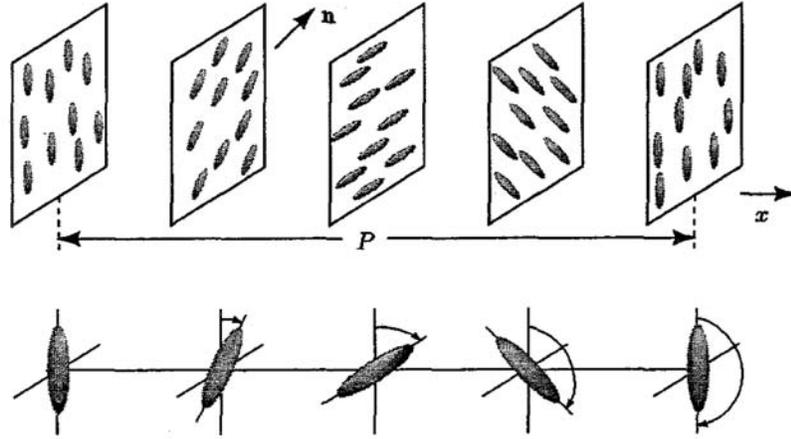
Figure 1.3: Cholesteric phase: This phase is composed of molecules which contain chirality. We see in the figure that a global chiral axis is established; this is the pitch. Along every location on the axis a perpendicular layer is established in which the molecules are aligned along a local director. The director rotates around the pitch in a helical pattern proportionally to the strength of the pitch.

planes direction. Applying the above convention it sets the director to lie in $\hat{z}$, $\hat{n} = (0, 0, 1)$. Since the centers of mass of the molecules are modulated in the $\hat{z}$ direction, the translational invariance is broken in that direction. However, in the $\hat{x}, \hat{y}$ directions still a two dimensional isotropic liquid exists. In the *de Gennes* description, the *SmA* phase can be treated as the equivalent to the state of a superconductor.

1.5   What is a topological defect?

Topological defects appear in coexistent phases, which include an order parameter as well as an external destructive field. A topological defect results from the breakdown of some symmetry. When the order parameter describes a superconductor, and a magnetic field is introduced those defects are vortices. Intuition can be supported when we think about the effect produced by a pointlike electron which introduces an infinite electric field.
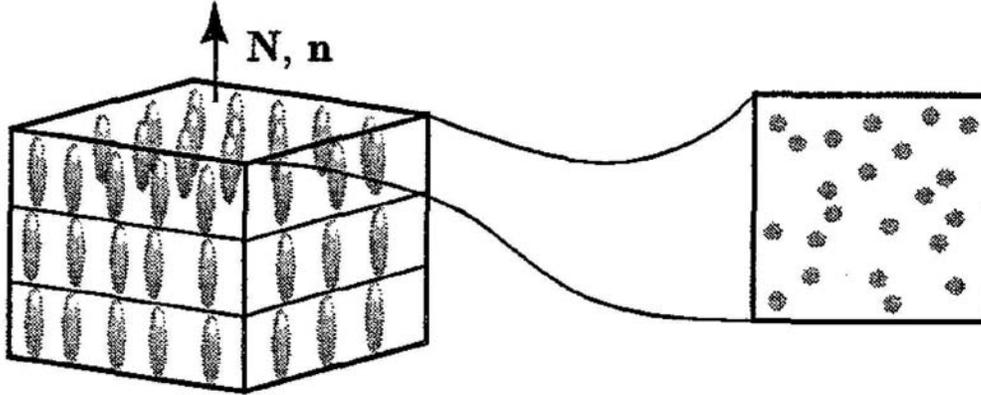
Figure 1.4: Smectic A Phase: The figure shows that the molecules in this phase are ordered in density layers. The molecules are not free to move in a three dimensional space, they are constrained to the x-y layer plane. Their axes are aligned with a director that is perpendicular to the layers plane. In the right figure a bird view is seen. It shows that in two dimensions the molecules are scattered arbitrary.

1.5.1   Vortices

A vortex results from the breakdown of the phase symmetry, it allows to introduce magnetic flux into the system.

1.5.2   Screw dislocations

In SmA, singularities are screw dislocations. A 2π rotation around the core lifts the planes by an integer multiple of the plane separation distance d. It is the breakdown of the modulated symmetry which also in SmA is expressed through the phase of the order parameter. Screw dislocations introduce a twist field into the SmA phase $\nabla_\perp \times q_s \delta \mathbf{n}_\perp$. They have the form of the magnetic field $\nabla \times \mathbf{A}$, their structure is of a staircase which lifts the planes in an integer multiple m of the distance between planes d, after every 2π rotation. m is the winding number. This is expressed in the following form $u = \frac{d}{2\pi}\phi(x,y) = \frac{d}{2\pi}\arctan(\frac{y}{x})$. u is the dislocation of a layer, for the following expression of the layers spatial orientation $z - u(\mathbf{x}) = md$. The screw dislocations in SmA are analogous to vortices in superconductors.
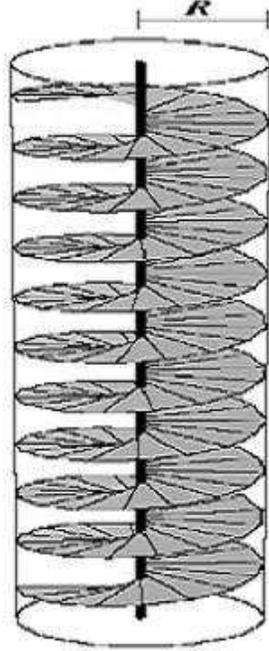
Figure 1.5: A Screw Dislocation in a layered material is a defect: It has a core around which it twists and lifts the layers in a helical pattern having the shape of a staircase. The radius of a dislocation is the radius beyond which the molecules are relaxed to their origin directions in the samples.

1.6 The Frank Oseen free energy

$$F_{nematic} = \frac{1}{2} \int K_1 (\boldsymbol{\nabla} \cdot \boldsymbol{n})^2 + K_2 (\boldsymbol{n} \cdot \boldsymbol{\nabla} \times \boldsymbol{n})^2 + K_3 (\boldsymbol{n} \times \boldsymbol{\nabla} \times \boldsymbol{n})^2. \quad (1.26)$$

This expression describes the strain energy of a phase, composed of molecules that have a director $\hat{\mathbf{n}}$, which are substituted to a mechanical stress. The terms appearing in (1.26) are: splay, twist and bend (see picture 1.6). It means that the strain energy tensor of such a samples bulk can always be diagonalized to the above form.

When the SmA phase is in equilibrium bend, twist and splay are expelled since they involve the increase of energy.

splay	twist	bend
$\vec{\nabla} \cdot \vec{n}$	$\vec{n} \cdot \vec{\nabla} \times \vec{n}$	$\vec{n} \times \vec{\nabla} \times \vec{n}$
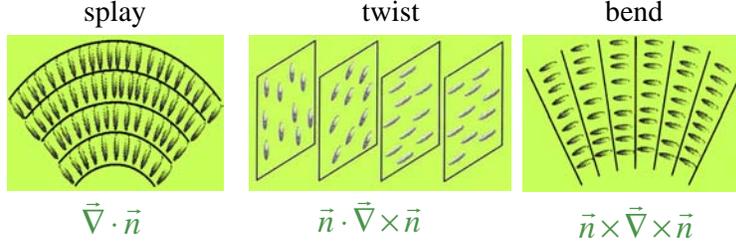
Figure 1.6: The Frank Oseen terms: (1) The splay term is due to bending of the layers around a core in a way that keeps the distance between them constant. Each layer is bent relative to its distance from the core so that the molecules have a radial orientation which is described mathematically by a divergence term. (2) The twist term is due to a bend core which passes through the layers perpendicularly and thus twists the layers around it. This breaks the alignment of molecules perpendicular to layers. (3) The bend term describes a bend around a core in a way that leaves the layers straight and increases the distance between them proportionally to the distance from the core. The molecules are then oriented tangentially.

1.6.1 The cholesteric free energy

In a *cholesteric* state, because of the form of the added chiral molecules, an internal twist is introduced to the sample. This is expressed by adding an energy term which minimizes the energy for a non zero twist. The Gibbs free energy therefore becomes

$$G_{chol} = F_{nematic} - k_2 \boldsymbol{k_0} \int d^3x (\boldsymbol{n} \cdot \boldsymbol{\nabla} \times \boldsymbol{n}). \tag{1.27}$$

In equilibrium $\boldsymbol{n} = \boldsymbol{n_0(y)} = (\sin k_0 y, 0, \cos k_0 y)$. $\boldsymbol{k_0} = k_o \hat{y}$ is the pitch wave number that is set to lie along the $\hat{y}$ axis. The following chiral field is defined $\boldsymbol{h} \equiv k_2 \boldsymbol{k_0}$.

1.7 The de Gennes free energy expression

In (1.25) we see that ρ_1 is the first harmonic of a modulated density and that φ is an arbitrary phase. In the *nematic* phase $\rho_1 = 0$, this is the reason for ρ_1 to be a logical choice for the *de Gennes* order parameter of the SmA phase. The condensation of the SmA is in the orientation of the center of mass of the molecules. The choice between the $\pm \hat{z}$ molecule orientations makes no difference, therefore a free energy describing the SmA phase may

be expanded in even powers of ρ_1. The fluctuations of the SmA layers are also considered by changing $\varphi \rightarrow \varphi(\mathbf{r}) = -q_s u(\mathbf{r})$ and $\rho_1 \rightarrow \rho_1(\mathbf{r})$, here $u(\mathbf{r})$ is the spatial dislocation of the layers. De Gennes proposed to combine those two features in order to define an order parameter for the SmA phase $\Psi = \rho_1(\mathbf{r})e^{i\varphi(\mathbf{r})}$. He obtained a complex scalar order parameter like it is used by Ginzburg and Landau to describe the superconductor phase. The analogy was further developed, since the expression describing the superconductor free energy was also an expansion of even powers of the order parameter. It is thus possible to follow a very similar process to analyze the properties of the *nematic* to SmA transition. The free energy describing the transition is:

$$
F_{SmA} - F_{nematic} = \frac{1}{2} \int r|\Psi|^2 + \frac{g}{2}|\Psi|^4 + C_\| |\frac{\partial \Psi}{\partial z}|^2 + C_\perp \left(|\frac{\partial \Psi}{\partial x}|^2 + |\frac{\partial \Psi}{\partial y}|^2 \right).
$$
(1.28)

The terms with $c_\perp$ and $c_\|$ were added to describe the energy involved with a spatial change of the order parameter in the perpendicular and parallel direction accordingly. It was needed to differ between those terms since in the parallel to the director's direction, perpendicular to the layers, the energy involved is different (usually higher) than in the perpendicular direction. Those terms express the tendency of the SmA to remain in its modulated order. The energy in (1.28) is typical for a second order transition since it is composed of even power terms. It is also necessary to take into account and add to (1.28) small fluctuations of the director from the $\hat{z}$ direction. Only fluctuations which are restricted to the $\hat{x} - \hat{z}$ plane are considered, so that $\hat{n} = (\sin\theta, 0, \cos\theta) \approx (\delta\hat{n}_\perp, 0, 1)$ where $\delta\hat{n}_\perp = \hat{n} - \hat{z}$ is defined. For small fluctuations, $n_z \approx 1$ and $\delta\hat{n}_\perp = \delta n_x \hat{x}$, without loss of generality. Therefore the energy does not change in the $\hat{z}$ direction. However, in order to compensate $C_\perp \left(|\frac{\partial \Psi}{\partial x}|^2 + |\frac{\partial \Psi}{\partial y}|^2 \right)$, in a way that leaves it proportional to the energy that is suited to the energy of the perpendicular direction to $\hat{n}$, it is needed to change the expression into the following:

$$
C_\perp \left(|\frac{\partial \Psi}{\partial x}|^2 + |\frac{\partial \Psi}{\partial y}|^2 \right) \rightarrow C_\perp |(\boldsymbol{\nabla}_\perp - iq_s\delta\hat{n}_\perp)\Psi|^2,
$$
(1.29)

where $\boldsymbol{\nabla}_\perp \equiv (\frac{\partial}{\partial x}, \frac{\partial}{\partial y})$ and q_s is the modulation density wave number. This form of an energy functional is typical for a gauge invariant term, as well as for superconductors. However, unlike in superconductors in SmA, the phase is a completely real and measurable quantity. To analyze the $SmA \leftrightarrow nematic$ transition, the Frank Oseen elastic free energy contribution is added, so that

in general we obtain

$$
\begin{aligned}
F_{SmA} \;=\; & \frac{1}{2}\int r|\Psi|^2 + \frac{g}{2}|\Psi|^4 + C_\parallel|\frac{\partial\Psi}{\partial z}|^2 + C_\perp|(\boldsymbol{\nabla}_\perp - iq_s\delta\hat{n}_\perp)\Psi|^2 + \\
+ \; & \frac{1}{2}\int K_1(\boldsymbol{\nabla}\cdot\boldsymbol{n})^2 + K_2(\boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n})^2 + K_3(\boldsymbol{n}\times\boldsymbol{\nabla}\times\boldsymbol{n})^2. \,(1.30)
\end{aligned}
$$

We see that for $\Psi = 0$ the SmA phase disappears, whereas if $\hat{n} = (0,0,1)$ the Frank expression disappears. The phase is determined by considerations of minimization of the total energy. If only the twist part in $F_{nematic}$ is considered, we get:

$$
\begin{aligned}
F_{SmA} \;=\; & \frac{1}{2}\int d^3x\{r|\Psi|^2 + \frac{g}{2}|\Psi|^4 + C_\parallel|\frac{\partial\Psi}{\partial z}|^2 + C_\perp|(\boldsymbol{\nabla}_\perp - iq_s\delta\hat{n}_\perp)\Psi|^2\} \\
+ \; & \frac{1}{2}\int d^3x\{K_2(\boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n})^2\}. \hspace{5cm} (1.31)
\end{aligned}
$$

This equation is very similar to the Ginzburg-Landau equation for superconductors and this is the reason for the comparison between those completely different physical systems. We can compare Ψ to the superconductor order parameter, $\delta\hat{n}_\perp$ can be compared to $\mathbf{A}$ the vector potential. The twist Frank Oseen energy term can be compared to the magnetic inductance $\mathbf{B} = \nabla\times\mathbf{A}$, and the parameters of those terms are compared respectively. However, there are some differences: First there are two extra Frank Oseen terms which do not exist in superconductors, second there is no $C_\parallel$ term in superconductors because the m^{-1} parameter appearing in superconductors is homogenous in all directions. Third, asymmetries arise because $\hat{n}_\perp$ and $(\boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n})^2$ are really two dimensional whereas $\mathbf{A}$ and $\mathbf{B}$ are three dimensional vectors. And finally the phase of the order parameter in SmA is purely real whereas in superconductors it is imaginary in general. Still there is much insight on the $nematic \rightarrow SmA$ transition from the above analogy.

1.8   The TGB phase

To continue the analogy first made by *de Gennes*, *Renn and Lubensky* proposed a theory for the existence of an analog to the Abrikosov state called 'Twist Grain Boundary' (TGB), which lies between the Meissner SmA state and the *nematic* phase. In this state the condensation of screw dislocations (topologically similar to vortices) is possible. The TGB phase was observed a short time later in an experiment by Goodby et al [14].

1.8.1 Description of the TGB phase

The TGB phase is build out of small Smectic A grains, each of length l_b. The grains are ordered along a pitch and turn around it in a helixlike pattern. The grains are separated from each other by a boundary which contains parallel screw dislocation lines. The dislocation lines are aligned parallel to the normal of the bordering grain layers. Inside the boundary the dislocations are separated by a distance of l_d from each other. Such boundaries exert a mean twist on the following grain which turns their layer normal by an angle of $2\pi\alpha$ relative to the previous normal direction (i.e. the normals are twisted by an angle of $2\pi\alpha$). The distance between two consecutive layers is d, so that the amount of twisting between grains is determined through the following formula $2\pi\alpha = 2\arctan(d/2l_d)$. If $\alpha \approx \frac{d}{2\pi l_d}$ is rational, there would be two different grains with repeating slab normals, and therefore the TGB phase would be a quasi crystalline, otherwise it is incommensurate. For a given strength of external twist field $K_2 K_0$, the angle created between consecutive grains and thus between directors inside them along the pitch is always smaller than the angle that would be created between directors separated the same distance in a Cholesteric phase. For a pitch along the $\hat{y}$ direction, the change of angle is presented as some function along the same axis $\frac{d\theta(y)}{dy}$. $K_2 k_0$ is analogous to an external magnetic field H. The magnetic flux density that penetrates a superconductor of the second kind is also smaller than the magnetic flux density that penetrates a normal phase which is surrounded by the same external field.

1.8.2 The Renn and Lubensky covariant free energy

It is not possible to explain the TGB phase through the de Gennes expression of the free energy because it assumes only small deviations of the director from a specific spatial direction through out the whole sample, say $\hat{z}$. Therefore, Renn and Lubensky have suggested a generalized free energy expression that can deal with larger deviations of n, and in fact does not have one spatial mean reference direction, but different ones with different directions changing spatially. Here we shall try to explain the main features of the Renn and Lubensky new covariant free energy expression. A specific system is studied, in which a SmA sample is placed in a way that its equilibrium director N lies along the $\hat{z}$ direction and the pitch of an external twist field is $\mathbf{p} = p\hat{y}$. For such a specification the force exerted on the director turns it around the pitch but leaves it in the $\hat{x}, \hat{z}$ plane. It is assumed that no other force fields exist in different spatial directions. All other vibrations are also disregarded as they are on average negligible. Under those assumptions, the director will
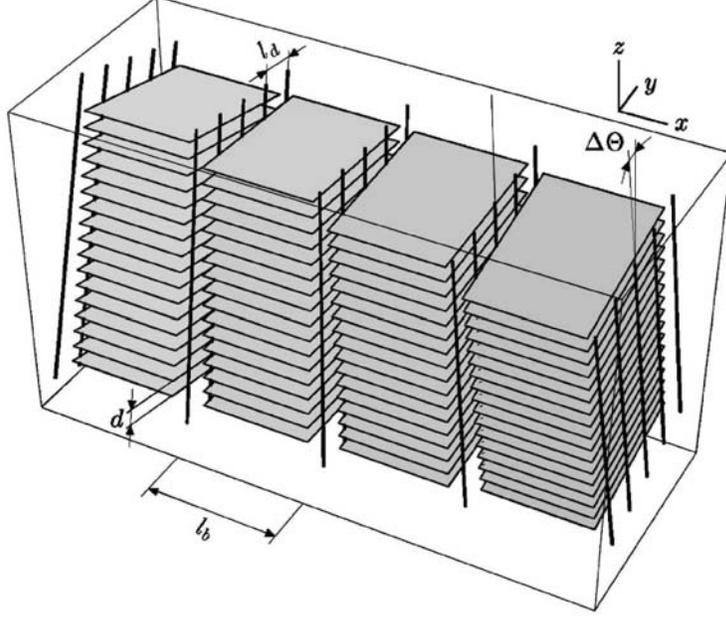
Figure 1.7: The TGB Phase in this picture follows a pitch which lies in the x axis direction. It is composed of SmA grains with inter-layer distance of d. The angle between consecutive grains of SmA is $\Delta\Theta = 2\pi\alpha$. The grains length is ℓ_b along the pitch. Between grains an array of parallel screw dislocations reside perpendicular to the bordering layer planes. The dislocations in each array are separated by ℓ_d.

always lie in the $\hat{x}, \hat{z}$ plane. It is then possible to use the following form for the director $\mathbf{n(y)} = (\sin\theta(\mathbf{y}), 0, \cos\theta(\mathbf{y}))$, where for the time being it is not known how $\theta(\mathbf{y})$ behaves. In a pure cholesteric the function $\theta(\mathbf{y})$ is simply equal to $k_0\mathbf{y}$, where k_0 is a constant which determines the strength of the pitch. For such a directional constellation in an intermediate zone between a cholesteric and a SmA Phase, the only non zero term of the Frank functional is the twist term. It is assumed that no other contributions arise from the bend and the splay terms. The following free energy is obtained:

$$
\begin{aligned}
F_{SmA} &= \int d^3x \{r|\Psi|^2 + \frac{g}{2}|\Psi|^4 + C_\parallel|\frac{\partial\Psi}{\partial z}|^2 + C_\perp|(\boldsymbol{\nabla}_\perp - iq_s\delta\hat{n}_\perp)\Psi|^2\} + \\
&+ \frac{1}{2}\int d^3x \{K_2(\boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n} - k_0)^2 - k_2 k_0^2\}.
\end{aligned} \tag{1.32}
$$

This is the form of the free energy that Renn and Lubensky used. It differs from the de Gennes form since a $\frac{1}{2}$ appears ahead of the twist term. This means that K_2 is twice as big in this formulation. We see that in fact the Frank elastic term is two-dimensional and that it is dependent on just its spatial location along the $\hat{y}$ axis since $\mathbf{n}$ behaves similarly. This can be written in the following manner:

$$
\begin{aligned}
F_{SmA} &= \int d^3x \{ r|\Psi|^2 + \frac{g}{2}|\Psi|^4 + C_\parallel |\frac{\partial \Psi}{\partial z}|^2 + C_\perp |(\nabla_\perp - iq_s \delta\hat{n}_\perp)\Psi|^2 \} + \\
&+ \frac{1}{2}\int d^3x \{ K_2(\nabla_y \theta - k_0)^2 - k_2 k_0^2 \}.
\end{aligned} \tag{1.33}
$$

However, the third and fourth term considering variation in the order parameter in the perpendicular and parallel directions to the director can not stay formulated as they are in the case of large variations in the angle of the director. It has to be defined in a way that will be corrected spatially and corresponding to the relative change in the direction of the director. This is the purpose of the following covariant form of the free energy expression by Renn and Lubensky:

$$
\begin{aligned}
F_{RL} &= \int d^3x \{ [(C_\parallel - C_\perp)n_i n_j + C_\perp \delta_{ij}][(\nabla - iq_s\mathbf{n})_i \Psi(\nabla - iq_s\mathbf{n})_j \Psi^*] + \\
&+ r|\Psi|^2 + \frac{g}{2}|\Psi|^4 \} + \frac{1}{2}\int d^3x \{ K_2(\nabla_y \theta - k_0)^2 - k_2 k_0^2 \}.
\end{aligned} \tag{1.34}
$$

This free energy can be understood in the following way: Instead of using $\delta\hat{n}_\perp = \hat{n} - \hat{z}$ which is good only for small fluctuations of the director around the $\hat{z}$ direction, it is needed to define the spatial equilibrium direction and to make everything relevant to it. First of all, it is important to mention that the order parameter has a slightly different form in this expression. Instead of taking only the first harmonic of the density vector, Renn and Lubensky took all its harmonic parts beginning from the first. Still it is clear that those harmonics play a role only for a SmA phase and are zero in the nematic phase and therefore are proper candidates for the order parameter. For i=j $[(C_\parallel - C_\perp)n_i n_j + C_\perp \delta_{ij}] \to C_\parallel$ and $\nabla \to \frac{\partial}{\partial i}$. The energy expression we obtain is the regular de Gennes energy expression for variations in the parallel direction. However, in this case changes of $\hat{n}$ can not be disregarded. These variations might be large which means that the assumption $\cos\theta \approx 1$ is not correct anymore. For $i \neq j$ we have in general $n_i n_j = sin\theta(y)cos\theta(y)$, which describes the amount of perpendicular energy $C_\perp$ and parallel energy $C_\parallel$ to be taken for the energy expression. In the cholesteric phase $\Psi = 0$ and $\nabla_y \theta = k_0$, so that the energy density is $f = -\frac{1}{2}k_2 k_0^2 = -\frac{h^2}{k_2}$. It can be compared to the

equilibrium energy density of a SmA $f = -\frac{1}{2}\frac{r^2}{g}$ in order to find the critical cholesteric field $h_c = \sqrt{\frac{k_2 r^2}{g}}$. This is the twist field strength equivalent to the critical magnetic field strength which breaks down the Meissner phase.

Chapter 2

Unique solutions of the free energy for an infinite two-dimensional superconductor

We return to superconductors reviewing the work of Akkermans and Mallick [2], in which they proposed an analytical way of obtaining directly from the Ginzburg-Landau free energy the existence of vortices. This was done by showing that the free energy points out solutions with inherent singularities of the order parameter in a two-dimensional infinite system and for a special point called the 'dual Point', whose definition will be explained in the second section of this chapter.

2.1   General dimensionless Ginzburg-Landau free energy

First, for a better understanding of the physical properties of the free energy we show that it is possible to write it in a dimensionless form using only the Ginzburg parameter κ. The Ginzburg-Landau free energy density (1.4) can be written in the following way:

$$f = a_0 + a_2|\Psi|^2 + a_4|\Psi|^4 + a_1\left|\left[\nabla - i\frac{2e}{\hbar c}A\right]\Psi\right|^2 + \frac{B^2}{8\pi}. \qquad (2.1)$$

Then $\alpha \equiv a_2, \frac{\beta}{2} \equiv a_4$ and $\frac{\hbar^2}{2m} \equiv a_1$. As a result the correlation length is $\xi^2 = \frac{a_1}{|a_2|}$. It compares the second term, which expresses the equilibrium of

the order parameter, with the the forth term, which expresses the spatial variation of the order parameter. The dimensions of the correlation length imposes that all terms have the dimensions of length. After dividing the free energy by $|a_2|$, the dimensions of $\left[\frac{a_1}{|a_2|}|\nabla\Psi|^2\right]$, $[|\Psi|^2]$ must be the same and thus the correlation square must be the compensation for the ∇^2 term, which is one over length square. The following properties have also been used: The flux quantum is $\frac{\phi_0}{2\pi} = \frac{\hbar c}{2e}$, the equilibrium of the order parameter is $\psi_0^2 = \frac{|a_2|}{2a_4}$ and and in the superconducting phase $\alpha \leq 0 \Rightarrow a_2 = -|a_2|$. All lengths are measured proportionally to the penetration length, $\sqrt{2}\lambda$. The magnetic density is measured in units of the quantum flux two-dimensional density (because the systems we study will be two-dimensional in character and the flux lines are perpendicular to it), so that $B_0 \equiv \frac{\phi_0}{2\pi r^2} = \frac{\phi_0}{2\pi(\sqrt{2}\lambda)^2} = \frac{\phi_0}{4\pi\lambda^2}$. The gradient is measured in $\nabla_0 \equiv \frac{1}{\sqrt{2}\lambda}$.

The dimensionality of the vector potential is obtained from $\nabla \times A = B$, and $\frac{\nabla}{\nabla_0} \times \frac{A}{A_0} = \frac{B}{B_0}$. We obtain $\nabla_0 A_0 = B_0 \Rightarrow A_0 = \sqrt{2}\lambda B_0 = \frac{\sqrt{2}\phi_0}{4\pi\lambda}$.

The penetration depth can be expressed as function of the parameters of the free energy. Like for the correlation length it can be derived from the comparison of the relevant terms, $\frac{B^2}{8\pi}$ and $a_1\left|\left[-i\frac{2eA}{\hbar c}\right]\Psi\right|^2$, both related to the magnetic field. The comparison of their dimensions is $\frac{A_0^2}{8\pi 2\lambda^2} = a_1(\frac{2e}{\hbar c})^2 A_0^2\psi_0^2$, which by inserting ψ_0 leads to $\lambda^2 = \frac{1}{8\pi}(\frac{\hbar c}{2e})^2\frac{a_4}{a_1|a_2|}$. However, since a_1 was determined to be $\frac{\hbar^2}{2m}$, as an artificial gauge for convenience it can be freely changed to set $\lambda^2 = \frac{1}{4\pi}(\frac{\hbar c}{2e})^2\frac{a_4}{a_1|a_2|}$. This will enforce the description of the dimensionless magnetic field to be $B'^2 \rightarrow \frac{1}{2}B'^2$, and the energy to be of its half size, which doesn't matter as the energy is a relative number.

The dimensionless free energy can now be written by inserting $\Psi = \psi'\psi_0$, $A = A'A_0$, $\nabla = \nabla'\nabla_0$ and $B = B'B_0$. The apostrophe denotes a dimensionless unit. Finally, in order to obtain a dimensionless energy expression it is divided with $\frac{B_0^2}{8\pi}$, then we obtain the following

$$\widetilde{F} = \int f = \int dV \left[\frac{1}{2}|B|^2 + \kappa^2(|\psi|^2 - 1)^2 + |(\nabla - iA)\psi|^2\right]. \qquad (2.2)$$

This is the dimensionless free energy, and since all variables are dimensionless we shall as of now (including (2.2)) drop all apostrophes. f is the dimensionless energy density and $\kappa^2 = \frac{\lambda^2}{\xi^2}$ is the square Ginzburg parameter, and the integration is over the volume V. As we can see, the energy is composed of a sum $(\kappa > 0)$ of three squared terms, so that it is either zero or positive. Both Ginzburg-Landau equations are derived by the method of variation.

The dimensionless equations are

$$(\nabla - iA)^2 \psi = 2\kappa^2 \psi(1 - |\psi|^2)$$
$$\nabla \times B = 2j \tag{2.3}$$

with the current density

$$j = Im(\psi^* \nabla \psi) - |\psi|^2 A. \tag{2.4}$$

The same boundary condition as in chapter 1 is used, naturally there is no current normal to the boundary of the superconductor (because it is surrounded with an insulator)

$$(\nabla - iA)\psi|_n = 0. \tag{2.5}$$

2.2 A special case of the free energy expression

The Ginzburg-Landau equations and expression (2.2) are valid for any system dimension. They are, however, non linear and therefore we do not know generally how to solve them to find their equilibrium. There is only one known exception. In this section we show that for two-dimensional systems and for the value $\kappa = \frac{1}{\sqrt{2}}$ called the dual point (because it is the Ginzburg parameter value separating a type I superconductor from type II superconductor), it is possible to derive an expression of the free energy which can be minimized.

A sample of a superconductor can be considered to be an effective two-dimensional superconductor if the thickness of its cross section in the direction of the applied magnetic field is small enough that neither the order parameter nor the magnetic potential change through it. For such a sample, all gradients perpendicular to the surface are zero and the only integrations of interest are in two dimensions. Let us derive the free energy expression that is suitable for a two-dimensional system lying in the $\hat{x} - \hat{y}$ plane and for a κ at the dual point:

$$\widetilde{F} = \int dA\{\frac{1}{2}|B|^2 + \frac{1}{2}(|\psi|^2 - 1)^2 + \tag{2.6}$$
$$+ (\nabla_x - iA_x)\psi\overline{(\nabla_x - iA_x)\psi} + (\nabla_y - iA_y)\psi\overline{(\nabla_y - iA_y)\psi}\}.$$

The overline denotes a complex conjugate term. The following is defined $D_m \equiv \partial_m - iA_m$; $m = x, y$, then

$$\widetilde{F} = \int dA \left[\frac{1}{2}|B|^2 + \frac{1}{2}(|\psi|^2 - 1)^2 + D_x\psi\overline{D_x\psi} + D_y\psi\overline{D_y\psi}\right]. \tag{2.7}$$

The Bogomol'nyi method provides an additional definition $D \equiv D_x + iD_y$. When $\mathbf{B}$ is inserted into the second term we obtain:

$$\widetilde{F} = \int dA [\frac{1}{2}(B + |\psi|^2 - 1)^2 - B(|\psi|^2 - 1) +$$
$$+ \ |D\psi|^2 + i\{D_x\psi\overline{D_y\psi} - D_y\psi\overline{D_x\psi}\}]. \tag{2.8}$$

The calculation of the curl of the current in two dimensions yields
$\nabla \times j = -B|\psi|^2 + i\{D_x\psi\overline{D_y\psi} - D_y\psi\overline{D_x\psi}\}$

$$\widetilde{F} = \int dA \left[\frac{1}{2}(B + |\psi|^2 - 1)^2 + |D\psi|^2\right] + \int \nabla \times [j + A]d\Omega. \tag{2.9}$$

The Stokes formula is used to obtain

$$\widetilde{F} = \int_{\partial\Omega} dA \left[\frac{1}{2}(B + |\psi|^2 - 1)^2 + |D\psi|^2\right] + \oint_{\partial\Omega} [j + A] \cdot d\mathbf{l}. \tag{2.10}$$

This is the Bogomol'nyi free energy expression. In this case the bulk part of the expression is the sum of just two positive terms. The minimum value for the bulk free energy corresponds to zero, which is yielded only if both positive terms vanish simultaneously and independently. In a two-dimensional system we have two variables of the order parameter. In conclusion, we have two equations for two variables. The Bogomol'nyi equation for the current is

$$\nabla \times j = -B|\psi|^2 + i\{D_x\psi\overline{D_y\psi} - D_y\psi\overline{D_x\psi}\} \tag{2.11}$$

and $j_m = Im(\psi^*\nabla_m\psi) - |\psi|^2 A_m$; $m = x, y$
which are the current terms in two dimensions.

2.3   The Bogomol'nyi identities and vortices as their solution

For an infinite superconducting disc at the boundary, $r \longrightarrow \infty$, the current $j \to 0$ and $\psi^2 \to 1$ and the boundary integral of (2.10) becomes

$$\oint_{\partial\Omega} [j + A] \cdot d\mathbf{l} \to \oint_{\partial\Omega} [\frac{j}{\psi^2} + A] \cdot d\mathbf{l}. \tag{2.12}$$

This is the expression of the London fluxoid. It is quantized and equal to $2\pi n$, for n which is the winding number of ψ. An extremum for $\widetilde{F}$ is obtained when the bulk term is equal to zero

$$D\psi = 0$$
$$B = 1 - |\psi|^2. \tag{2.13}$$

These are the Bogomol'nyi identities, when they are valid, the free energy is equal to $\widetilde{F} = 2\pi n$. The Bogomol'nyi identities can also be expressed differently. The first identity is written as follows,

$$[(\partial_x + i\partial_y) - i(A_x + iA_y)]\psi = 0 \tag{2.14}$$

then the following are defined $\overline{\partial} = \partial_x + i\partial_y$ and also $\overline{A} = A_x + iA_y$. They become the complex conjugates of $\partial = \partial_x - i\partial_y$ and $A = A_x - iA_y$ and the first identity becomes $[\overline{\partial} - i\overline{A}]\psi = 0$. The complex conjugate of that identity therefore is $\partial\overline{\psi} = -iA$. It is multiplied from the left with $\overline{\psi}$ and the second identity is multiplied by ψ. This yields

$$\begin{aligned} \overline{\psi}\partial\psi &= i\overline{A}|\psi|^2 \\ \psi\partial\overline{\psi} &= -iA|\psi|^2. \end{aligned} \tag{2.15}$$

The left hand side of these equations can be written in the following manner

$$\begin{aligned} \overline{\partial}|\psi|^2 - \psi\overline{\partial\psi} &= i\overline{A}|\psi|^2 \\ \partial|\psi|^2 - \overline{\psi}\partial\psi &= -iA|\psi|^2. \end{aligned} \tag{2.16}$$

Then they both are divided with $|\psi|^2$. Their derivative is

$$\begin{aligned} \partial\overline{\partial}\ln|\psi|^2 - \partial\overline{\partial}\ln\overline{\psi} &= i\partial\overline{A} \\ \overline{\partial}\partial\ln|\psi|^2 - \overline{\partial}\partial\ln\psi &= -i\overline{\partial}A. \end{aligned} \tag{2.17}$$

The right hand side of both equations are $-\mathbf{B}$ with an added term of $+i\nabla\cdot\mathbf{A}$ or $-i\nabla\cdot\mathbf{A}$. Further we observe that $\overline{\partial}\partial = \nabla^2$, so that adding both equations yields

$$\nabla^2\ln|\psi|^2 = -2B. \tag{2.18}$$

As a final step, the second Bogomol'nyi identity is inserted. The result that is obtained is an independent equation for $|\psi|^2$

$$\nabla^2\ln|\psi|^2 = 2(|\psi|^2 - 1). \tag{2.19}$$

This equation is known to be the Liouville equation, and there are solutions to it which can admit singularities in the order parameter field. For superconductors they are vortices. The number of quantum flux is given by the winding number n. The energy on the other hand is given by the same winding number $\widetilde{F} = 2\pi n$. However, the energy expression does not tell what should be the number n and it is a parameter which is determined by the system independently. Since there is the possibility that n is zero, the above is not even sufficient to show that vortices at all exist in the system. Still the

derivation shows analytically that the existence of vortices is theoretically possible, and therefore its importance. This result is another very important feature of the Ginzburg-Landau free energy for infinite superconductors.

It was shown by E.Akkermans and K.Mallik [2] that if the proper energy considerations are added to a system that has a boundary, it is possible to determine an exact number different from zero for the existing vortices. Herewith they showed that the existence of a boundary fixes a finite number for the winding number n. The objective of this thesis is to show the same features for liquid crystals SmA samples.

Chapter 3

A smectic A cylinder of infinite length and infinite radius

To this point we have described what is known previous to this work. This is the starting point for this thesis.

The system we consider is a SmA sample with the shape of a very long cylinder with its axis along the $\hat{z}$ direction. Here, we examine the case of a cylinder with an infinite radius. It has to be mentioned, however, that such a system cannot be physical if it contains screw dislocations. Sethna [21] has claimed that an infinite system containing screw dislocations would create infinite slopes to the SmA layers. However, we shall use the results of this chapter only for finite samples. Therefore, we can ignore the problem mentioned by Sethna. For this chapter, we shall use an infinite model containing screw dislocations to get some analytical results.

We start with the de Gennes free energy (in the Renn and Lubensky formulation).

$$
\begin{aligned}
F_{SmA} &= \int d^3x \{ r|\Psi|^2 + \frac{g}{2}|\Psi|^4 + C_\parallel |\frac{\partial \Psi}{\partial z}|^2 + C_\perp |(\boldsymbol{\nabla}_\perp - iq_s \delta\hat{n}_\perp)\Psi|^2 \} + \\
&+ \frac{1}{2}\int d^3x \{ K_2(\boldsymbol{n} \cdot \boldsymbol{\nabla} \times \boldsymbol{n})^2 \}
\end{aligned}
\tag{3.1}
$$

This energy form is only justified within the limitation of a director $\hat{n}$ making small vibrations around its equilibrium direction, which we define to be the $\hat{z}$ direction. The geometry of the problem is therefore one in which we have layers of SmA arranged along the $\hat{z}$ direction. This is a quasi two-dimensional geometry, since along the $\hat{z}$ direction there are no variations other than the SmA constant density modulation. It is already included in the definition of the SmA order parameter (i.e. q_s is constant and the order parameter is independent on it). This means that in the $\hat{z}$ direction the order parameter

is a single valued constant, and that it depends only on its $(\hat{x}, \hat{y})$ coordinates. Therefore it is a case of an infinite two-dimensional system.

3.1   The dimensionless free energy

In order to understand better the properties of the *cholesteric* $\rightarrow$ *SmA* transition, the free energy (3.1) can be rewritten as a function of only one dimensionless parameter which shall be defined.

The last term in (3.1),which denotes the twist, is rewritten so that it manifests the idea that the director is allowed to vibrate only slightly ($\boldsymbol{n} \cdot \boldsymbol{\nabla} \times \boldsymbol{n})^2 \rightarrow (\nabla_\perp \times \delta\mathbf{n}_\perp)^2$. Because no forces are applied in the $\hat{z}$ direction, the term $C_\parallel |\frac{\partial \Psi}{\partial z}|^2$ is a constant of the energy and is dropped. Let us now write the energy expression the way we did it for superconductors:

$$
\begin{aligned}
F_{SmA} &= \int d^3x \{ a_2 |\Psi|^2 + a_4 |\Psi|^4 + C_\perp |(\boldsymbol{\nabla}_\perp - iq_s\delta\boldsymbol{n}_\perp)\Psi|^2 + \\
&+ \frac{1}{2} K_2 (\nabla_\perp \times \delta\mathbf{n}_\perp)^2 \}.
\end{aligned}
\tag{3.2}
$$

Where the following: $a_2 \equiv r$, $a_4 \equiv \frac{g}{2}$, $a_1 \equiv C_\perp$ have been used. At this point the perpendicular coherence length $\xi_\perp$ of (3.2) can be defined. It is the first characteristic length of the energy and denotes the length over which the *SmA* order parameter changes in the (x,y) plane. $\xi_\perp$ is obtained by comparing the perpendicular gradient term with the first term in the energy functional (3.2). This sets $\xi_\perp = \sqrt{C_\perp/|r|}$. To obtain a dimensionless expression for (3.2), the order parameter is written in units of its equilibrium value $\Psi = \psi_0\psi = \sqrt{\frac{|a_2|}{2a_4}}\psi$. All lengths are measured in units of $\sqrt{2}\lambda$. The units of the gradient are then expressed as follows: $\nabla_\perp^0 = \frac{1}{\sqrt{2}\lambda}$. And the units of the density wave vector become $q_s^0 = \frac{1}{\sqrt{2}\lambda}$. When inserted into (3.2), they yield:

$$
\begin{aligned}
f &= \frac{|a_2|^2}{4a_4}(|\psi|^2 - 1)^2 - 1 + \frac{a_1|a_2|}{2a_4}\frac{1}{2\lambda^2}|(\nabla_\perp' - iq_s'\delta\mathbf{n}_\perp)\psi|^2 + \\
&+ \frac{K_2}{2\lambda^2 q_s'^2}\frac{1}{2}(\nabla_\perp' \times q_s'\delta\mathbf{n}_\perp)^2
\end{aligned}
\tag{3.3}
$$

f is the energy density. $q_s', \nabla_\perp'$ denote a dimensionless density wave number and gradient. When the last term in (3.3) is multiplied and divided by $q_s'^2$, it is then analogous with the second term of the energy density expression for superconductors. Clearly $q_s\delta\mathbf{n}_\perp$ is then the equivalent to the vector potential **A**.

The expression turns out to be dimensionless when it is divided by $\frac{K_2}{2\lambda^2 q_s'^2}$, which has the dimensionality of energy. The penetration length which is the second characteristic length is defined in a way similar to that of a superconductor. This is possible due to the analogy between the expressions of their free energy. The appropriate terms are compared in the energy expression and yield: $\lambda^2 = \frac{a_4 K_2}{a_1 |a_2| q_s^2} = \frac{g K_2}{2 C_\perp q_s^2 |r|}$. λ denotes the distance over which a change in direction perpendicular to the director field in the SmA can occur. For this expression, the director would tilt away from its equilibrium direction at the boundary only due to an external applied twist field. Therefore, it is named twist penetration length and will be denoted λ_T. Two characteristic lengths have been identified, the correlation length and the penetration length. Since their temperature dependence is equal (they depend on the same mean field temperature parameters) we can define a dimensionless parameter $\kappa = \frac{\lambda_T}{\xi_\perp}$. This is the Ginzburg parameter which is temperature independent and therefore a characteristic constant describing the material. The dimensionless energy expression is then rewritten to express that it depends only on the Ginzburg parameter.

$$f = \kappa^2 (|\psi|^2 - 1)^2 + \frac{1}{2}(\nabla_\perp \times q_s \delta\mathbf{n}_\perp)^2 + |(\nabla_\perp - iq_s \delta\mathbf{n}_\perp)\psi|^2 \qquad (3.4)$$

Expression (3.4) is the dimensionless free energy density, describing the phase transition between the SmA phase and the nematic phase. Since from this point further we shall only discuss dimensionless equations, all apostrophes are dropped. The second term of (3.4) is the energy from the twist field which will be denoted by $\boldsymbol{\tau}(\mathbf{r}) \equiv \nabla_\perp \times q_s \delta\mathbf{n}_\perp$. The third term is of the form of a generalized momentum for the SmA order parameter. If instead of a nematic a cholesteric phase was existent, the twist term of the free energy expression would have been changed to $\boldsymbol{\tau}(\mathbf{r}) - q_s k_0$. In this case, the system is in equilibrium when it exhibits a finite twist and for $\psi = 0$. But in the smectic phase, $\psi \neq 0$, and a twist induces the increase of energy. Therefore, the twist vanishes at equilibrium at distances larger than the twist penetration length. There is an energy competition between the twist energy and the smectic energy. We can think of the nematic phase as analogous to a metal and of the Smectic phase as analogous to a superconductor; the cholesteric phase would then be analogous to a metal exposed to an applied magnetic field. It seems that for a large enough twist field a second order phase transition, which turns the SmA to a cholesteric phase, should occur. This is, however, only partially correct when $\kappa < \frac{1}{\sqrt{2}}$, but for values of $\kappa > \frac{1}{\sqrt{2}}$ we shall expect a type II SmA phase similar to type II superconductors. A type II SmA phase should contain topological defects similar to the appearance of vortices in superconductors.

3.2 Bogomol'nyi equations and a topological solution

We recognized that equation (3.4) is exactly similar to equation (2.2) and that the second term in (3.4) can be compared to the magnetic field term in (2.2), but only when the systems are two-dimensional. This means that in contradiction to the magnetic field term in the Ginzburg-Landau free energy for superconductors, the twist field term in the Ginzburg-Landau free energy for SmA must have a two-dimensional symmetry. For $\kappa = \frac{1}{\sqrt{2}}$ at the 'dual point', the procedure from chapter 2 to obtain the Bogomol'nyi identities can be used but only as long as the twist field is in the direction of the cylinder axis. Under this condition, the system in question is a two-dimensional Ginzburg-Landau system at the 'dual point', and it is possible to separate the free energy into a bulk and a boundary integral:

$$F = \int_{\Omega} d\Omega \left[\frac{1}{2} (\boldsymbol{\tau} + |\psi|^2 - 1)^2 + |D\psi|^2 \right] + \oint_{\Gamma} [j + q_s \delta \mathbf{n}_\perp] \cdot d\mathbf{l}. \qquad (3.5)$$

The bulk is composed of two independent positive defined terms which vanish for the minimization of the free energy. They vanish when the following liquid crystals Bogomol'nyi identities stand:

$$\begin{aligned} D\psi &= 0 \\ |\boldsymbol{\tau}(\mathbf{r})| &= 1 - |\psi|^2. \end{aligned} \qquad (3.6)$$

Then it is also possible to obtain the Liouville equation for the SmA order parameter

$$\nabla^2 \ln |\psi|^2 = 2(|\psi|^2 - 1). \qquad (3.7)$$

As discussed in the previous chapter, the Liouville equation admits solutions with singularities. When the order parameter vanishes and nematogen molecules can 'jump' to a different layer the existence of a screw dislocation is also enabled.

3.3 Interpretation of the solution

In the previous section we have seen that the free energy of a SmA can be written as a sum of a bulk term and a boundary term. The minimization of this free energy requires the bulk term to disappear. The condition for the vanishing of the bulk leads to the Liouville equation for the order parameter field. The solutions of the Liouville equation describe an order parameter

field which contains singularities. The second part of the free energy is a boundary term and as such it varies correspondingly to the specifically defined boundary conditions.

First a simple case is analyzed, the case of a boundary which lies at infinity i.e. there is no boundary. To minimize the free energy of such a system, some simple assumptions are made that allow to calculate the boundary integral:

1. We assume that at infinity the order parameter relaxes to its equilibrium value ($\psi_0 = 1$).

2. We assume that at infinity no currents exist ($\mathbf{j} = 0$).

Under those conditions we can write:

$$\oint_\Gamma [j + q_s \delta \mathbf{n}_\perp] \cdot d\mathbf{l} = \oint_\Gamma [\frac{j}{|\psi|^2} + q_s \delta \mathbf{n}_\perp] \cdot d\mathbf{l} = \oint_\Gamma [\nabla_\perp \varphi] \cdot d\mathbf{l} = 2\pi\ell. \qquad (3.8)$$

This expression is similar to the London fluxoid in superconductivity, it expresses the quantization of twist flux inside of a SmA. For a superconductor the flux is quantized because the superconductor order parameter is made to be single valued. This is also the case for the SmA order parameter, as the order parameter must have a physical interpretation. There is one remark that must be added: In contrast to the phase of the superconductor order parameter which is not a measurable (only differences of the phase can be measured), the phase of the SmA is an absolute measurable quantity, but this does not alter the fact of quantization. The result of a quantized flux inside a SmA sample is the lifting of layers in a stepwise way, in units of layer separation distances. If we follow a plane circulating a screw dislocation with flux strength $2\pi\ell$, then after one circulation there is a lift to a plane which is $\ell \times d$ higher or lower from the plane beginning with (see 1.5). d is the distance separating consecutive SmA planes.

$$h_l = h_0 + d \times \ell \qquad (3.9)$$

To conclude the case of no boundary for a two-dimensional SmA at the 'dual point'($\kappa = \frac{1}{\sqrt{2}}$), it is possible to divide the free energy to a bulk and an edge integral (the Bogomol'nyi method). Minimization of the free energy is achieved by applying the Bogomol'nyi equations on the bulk terms which makes them disappear. It also leads to the Liouville equation for the order parameter field, which solutions are known to have families of topological dislocations. On the other hand, because the boundary is at infinity, we can treat the boundary integral as a fluxoid and we obtain that the free energy

is topological and depends on the integer number ℓ counting the amount of flux quanta existing in the system

$$F = 2\pi\ell. \tag{3.10}$$

This case shows that the free energy is dependent on the amount of screw dislocations. However, it does not reveal how many such dislocations exist in a system, since ℓ is an independent number. Furthermore there is no indication in this result why a system should prefer a certain number ℓ of screw dislocations over another, or what physical considerations effect it.

For superconducting billiards the answer to those questions were provided by E. Akkermans and K. Mallick [2]. In the next chapter it will be shown how to apply their method to SmA samples.

Chapter 4

A mesoscopic *SmA* cylinder

In this chapter it is shown that when a SmA system has a boundary, the choice of appropriate boundary conditions leads to a selection mechanism for the number of screw dislocations. This is the case of a system in the form of an infinite long cylinder with a finite radius length R.

The cylinder axis is set to lie in the $\hat{z}$ direction, parallel to the direction of the SmA layers. This symmetry sets the SmA order parameter to be two-dimensional. Our theory is only valid when the radius is limited between a maximum and a minimum size. We shall call such a system a mesoscopic system. The solution of the problem of finite size samples however can not be similar to the infinite case, since for such systems the Bogomol'nyi bound does not exist (the boundary integral can not be expressed to be the fluxoid).

4.1   The boundary conditions

First it is necessary to set a few assumptions for a SmA system.

1. The radius is set to be $\frac{1}{2}R > \xi_\perp \cong \lambda_T$ (a more precise inequality will be given later).

2. The changes of the director are assumed to be small $\delta\mathbf{n}_\perp << 1$. This implies that only a small number of induced screw dislocations ℓ in the system is allowed, and that the radius is not larger than $R << \frac{2\pi}{k_0}$.

3. The assumptions above set a rough approximation for the allowed radius of the cylinder which we call the mesoscopic limit.

4. The existence of a material with $\kappa = \frac{1}{\sqrt{2}}$ is assumed.

5. It is assumed that the SmA sample can accommodate a twist flux through it, that is bounded by: $\Phi_{LP} = \frac{\Phi_{SmA}}{2\pi} = \frac{R^2 k_0}{2}$.

6. Induced screw dislocations, lie in the center of the sample.

7. There are no edge dislocations.

The second assumption is necessary since the de Gennes free energy is only valid for small variations around the director's mean direction. The fifth assumption is unnecessary if the second is valid, it only states that for the liquid crystal material chosen, the mean field theory is valid, and that the applied twist field only produces small changes in the director. It will be shown that this assumption is self contained in assumption number two. The last assumption is plausible for the cylindrical geometry that was set for the sample. As an example we shall study a sample that contains one screw dislocation and an external surrounding twist field. For that case the following stands:

1. The twist flux through the screw dislocation is in the direction of the external induced twist.

2. The external twist field penetrates the edge of the sample up to a distance of the penetration depth δ.

The second statement is the famous Meissner effect for the SmA phase. It is simple to show that the Meissner effect is valid for any material that can be described within the framework of the Ginzburg-Landau theory (see (1.12)).

It implies that the SmA sample induces edge currents that screen the external field out. Those screening currents flow in a direction that corresponds to a circulation (according to the right hand rule), which is opposite to the external twist field.

The first statement is obvious, and it implies that currents surrounding the core of the twist dislocation flow in a direction that corresponds to a circulation along the direction of the external twist field. Furthermore, the center current as well as the edge current are tangential since the symmetry of the system, the direction of the external twist field are cylindrical and since it is assumed that the dislocation lies in the center. This assumption is based on the observation that topological defects in superconducting billiards at the dual point with radial symmetry will usually lie in the center [3]. In conclusion, the edge and the bulk currents will flow in opposite directions. Therefore we see that the existence of a sample corresponding to this theory is conditioned with a minimum system radius which can absorb both currents.

Then a closed contour in the sample around the center with zero current circulation (and in our case this implies zero current) must be found in the sample. It is therefore possible to define a center bulk area and an edge

area separated by direction of the currents that flow in them. A picture that describes the above example is presented in figure (4.1). It shows a sample containing a dislocation in its center and a twist field surrounding it.
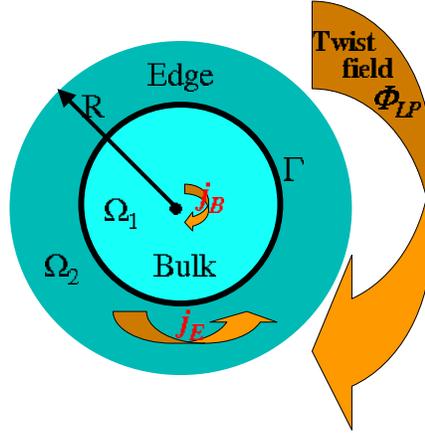

Figure 4.1: In this figure we can see a sample of radius R on which an external twist Φ_{LP} is exerted. The external twist field is too strong to be screened out by the edge currents, and a screw dislocation is introduced into the center. It causes bulk currents around it that flow in an opposite direction to the edge currents. The sample can be divided into a bulk and an edge according to those currents. The separating contour Γ between those regions is defined to lie where the total circulation vanishes.

The core size of a topological defect is of the distance of the correlation length. This is the distance over which it takes the order parameter to relax to its equilibrium value in the bulk. Therefore, it is also the distance over which currents flow around the screw dislocation core. It shows that assumption number one is necessary to assure that the size of the sample will be large enough to contain the complete core. In fact numerical calculations of (1.4) for mesoscopic superconductor discs (see figure 4.2) have shown that a finite inter area appears. In this part, the order parameter is almost equal to its bulk value and the magnetic field disappears, hence no current circulation exists.

The existence of a zero current contour led Akkermans and Mallick to find a solution for the equilibrium of mesoscopic superconducting billiards by separating the free energy to a bulk region Ω_1, and an edge Ω_2 region. The free energy can then be approximated by:

$$\int_\Omega f d\Omega = \int_{\Omega_1} f_{\Omega_1} d\Omega + \int_{\Omega_2} f_{\Omega_2} d\Omega \qquad (4.1)$$
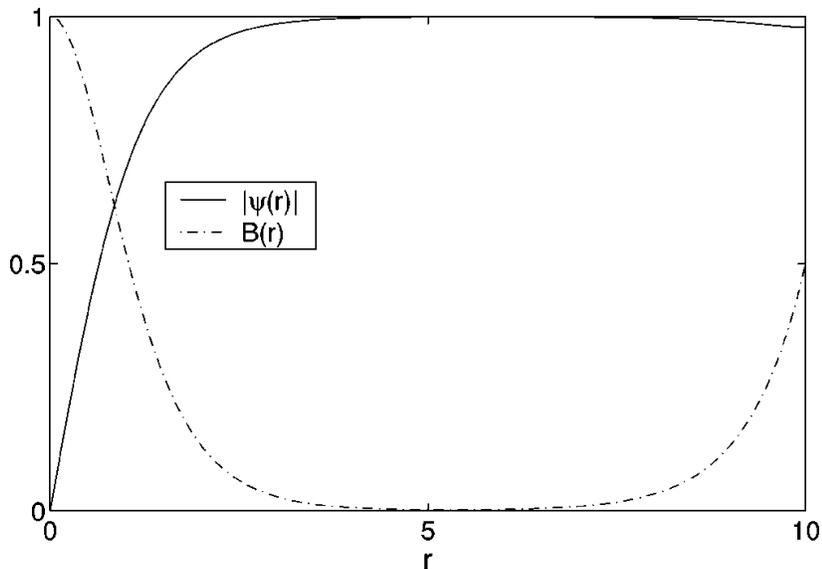
Figure 4.2: This graph shows a numerical calculation done for superconducting billiards with radius 10. It calculates the magnetic field and order parameter within a sample that contains one vortex in its center. They [3] used the complete form of the Ginzburg-Landau free energy expression 2.2 which is in complete analogy to expression 3.4. It is shown that in the vicinity of $R = 5$ the magnetic field vanishes and the order parameter relaxes to its equilibrium value. Near the boundary of the sample the magnetic field rises exponentially but the order parameter is decreased only moderately from its equilibrium value. At the center of the vortex the order parameter vanishes.

This is an approximation, since the order parameter is only approximately constant and equal to its bulk equilibrium value. This approximation also assumes that correlations between the currents of the bulk and the edge do not exist. However experimental data [3] has confirmed this approximation to be very good.

Since the bulk is separated from the edge by a zero current contour $\mathbf{j}|_\Gamma = 0$, the method of the infinitesimal sample case can be applied, so that the bulk energy is approximated to be the Bogomol'nyi bound. It is then given by:

$$\int_{\Omega_1} f_{\Omega_1} d\Omega \cong 2\pi\ell. \tag{4.2}$$

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4.2 The edge free energy

The edge region energy F_{Ω_2} is calculated from the general dimensionless free energy expression:

$$\int_{\Omega_2} f_{\Omega_2} \ d\Omega \ =$$
$$= \int_{\Omega_2} d\Omega \ \left\{ \frac{1}{2}(|\psi|^2 - 1)^2 + \frac{1}{2}(\nabla_\perp \times q_s \delta \mathbf{n}_\perp)^2 + |(\nabla_\perp - i q_s \delta \mathbf{n}_\perp)\psi|^2 \right\}. \tag{4.3}$$

The expression for the order parameter $\Psi = \psi e^{i\varphi}$ is inserted into the last term in order to decompose it:

$$\int_{\Omega_2} f_{\Omega_2} d\Omega =$$
$$\int_{\Omega_2} d\Omega \left\{ \frac{1}{2}(|\psi|^2 - 1)^2 + \frac{1}{2}(\nabla_\perp \times q_s \delta \mathbf{n}_\perp)^2 + (\nabla_\perp \psi)^2 + \psi^2 (\nabla_\perp \varphi - q_s \delta \mathbf{n}_\perp)^2 \right\}. \tag{4.4}$$

Since, according to the numerical calculation (see figure 4.2), the gradient of the order parameter in the edge region is very small compared to the other terms, it will be dropped.

Finally, the following is calculated:

$$\int_{\Omega_2} f_{\Omega_2} d\Omega =$$
$$= \int_{\Omega_2} d\Omega \left\{ \frac{1}{2}(|\psi|^2 - 1)^2 + \frac{1}{2}(\nabla_\perp \times q_s \delta \mathbf{n}_\perp)^2 + \psi^2 (\nabla_\perp \varphi - q_s \delta \mathbf{n}_\perp)^2 \right\}. \tag{4.5}$$

It is believed that it is possible to control in a specific system the edge defects, so that they become relatively negligible, and (4.5) is a correct first approximation, such that no added edge terms to the energy expression are needed. This point will be discussed furthermore at section 5.3.

To calculate expression (4.5), it is necessary to set boundary conditions. We choose to use the Little Parks method, applied to liquid crystals as a good way to find suiting boundary conditions.

To apply the Little Parks method for liquid crystals in a simple way, a convenient geometry of the twist field is defined with the following properties: It is a twist field that has a pitch in every radial direction (of a plane), and in all directions the twist wave vector is set to be of the same size of k_0. This field shall be called the "radial twist" field, and its twist flux will be denoted as Φ_{LP}. The "double twist" phase by Kamien [16] is a phase exhibiting very similar field properties to the "radial twist" field. It is a cholesteric phase

with two perpendicular pitch axes so that in every radial direction it has a pitch with a wave vector size that is a linear combination of them. The field defined is slightly more symmetrical and thus easier to calculate. A double twist phase would yield the same characteristics, but shift the numerical results, the main results will hold. As long as a zero circulation contour is established in the sample, the principle results will stand.

Such a "radial twist" field surrounding a SmA sample exerts a stress, leading the sample to twist around its axis.

The following figure (4.3) presents the situation we have described.
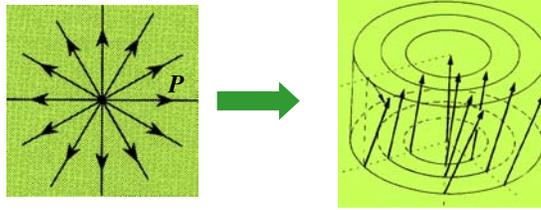
Figure 4.3: The left figure shows the case of what we call a Little Parks field, a twist field of radial pitch. On the right we show the resulting strain in a SmA cylindrical grain which is located in the center of the field. The arrows represent local SmA directors. We can see that they tilt increasingly in the tangential direction as the distance from the center grows. δn, which is the projection of $\mathbf{n}$ on the plane of the SmA layers, is therefore tangential and increases radially.

The Little Parks method for liquid crystals assumes that the total twist flux through a SmA sample is bounded by the twist flux accommodated by the same volume when no sample is inserted into the same external twist field, and that the field's radial pitch wave vector is k_0. In simple words it means that the twist flux through the SmA sample can only be less than or equal to the twist flux of the "radial twist" field.

$$\Phi_{SmA} = 2\pi\Phi_{LP} = \pi R^2 k_0 \qquad (4.6)$$

The symmetry of the case we have described will set $\delta\mathbf{n}_\perp$ to be tangential as it is depicted in figure (4.3). The current density will be as well tangential, and depend only on the distance from the center of the sample.

$$\delta\mathbf{n}_\perp = \delta\mathbf{n}_\perp(\mathbf{r})\hat{\Theta} \qquad \mathbf{j}_\Theta(\mathbf{r}) = \psi^2(\nabla_\perp\varphi - q_s\delta\mathbf{n}_\perp) \qquad (4.7)$$

Where $\hat{\Theta}$ is the tangential direction. The value of the twist flux in the sample is attained by integrating the twist term of the free energy over the complete

area of the sample, this yields:

$$\Phi_{LP} = \frac{q_s}{2\pi} \oint_{\partial\Omega} \delta\mathbf{n}_\perp \cdot d\boldsymbol{l} = Rq_s\delta n_\perp(R). \qquad (4.8)$$

Thus on the boundary of the sample we have

$$\delta\mathbf{n}_\perp(R) = \frac{k_0 R}{2q_s}\hat{\Theta}. \qquad (4.9)$$

The value of the phase on the boundary of a sample that contains ℓ screw dislocations corresponds to $\oint_{\partial\Omega} \nabla_\perp\varphi \cdot d\boldsymbol{l} = 2\pi\ell$. And therefore on the boundary we have:

$$\nabla_\perp\varphi|_{\partial\Omega} = \frac{\ell}{R}\hat{\Theta}. \qquad (4.10)$$

If (4.10) and (4.9) are inserted into (4.7) then, for

$$\ell \leq \frac{k_0 R^2}{2} = \Phi_{LP}, \qquad (4.11)$$

the current on the boundary is negative. And since around the core of the sample the current is positive, it is clear that in between the boundary and the bulk core, a closed contour must exist for which the current vanishes. This is therefore the limit that is set for the number of screw dislocations allowed in the sample. It allows the Bogomol'nyi bound to be a good approximation for the free energy of Ω_1.

When (4.11) is an equality, the zero current contour is found to be on the edge of the sample. There is no edge region and the complete energy of the sample is a result of the Bogomol'nyi bound. Moreover for such a configuration, there are no edge currents to screen the external field and the entrance of more dislocations into the sample is enabled. For ℓ smaller, there is a finite edge region Ω_2. If an external twist is applied, it penetrates the edge region and decays in it exponentially, relative to a distance of penetration depth that we denote δ. It is emphasized that in general $\delta \neq \lambda$. Since, λ is the characteristic mean field penetration depth for a system without a boundary, a different approach has to be taken to calculate δ. It is calculated to be such that it minimizes the free energy of Ω_2. We write:

$$\boldsymbol{\tau}(\boldsymbol{r}) = \boldsymbol{\tau}(R)e^{\frac{-(R-r)}{\delta}}, \qquad (4.12)$$

where $\boldsymbol{\tau}(R)$ denotes the twist field on the boundary of the sample. It can be calculated by implementing the boundary conditions on it . The complete twist flux is

$$\Phi_{LP} = \ell + \frac{1}{2\pi} \int_{\Omega_2} \boldsymbol{\tau}(\boldsymbol{r})d\Omega \approx \ell + R\tau(R). \qquad (4.13)$$

Inserting (4.13) into (4.19) gives

$$\boldsymbol{\tau}(\boldsymbol{r}) = \frac{\Phi_{LP} - \ell}{R} e^{\frac{-(R-r)}{\delta}} \hat{z}. \tag{4.14}$$

The following identities are used to calculate the free energy:

$$\frac{\boldsymbol{\nabla} \times \boldsymbol{j}(\boldsymbol{r})}{|\psi|^2} = -\boldsymbol{\tau}(\boldsymbol{r}) \tag{4.15}$$

$$\left\{\frac{\boldsymbol{j}(\boldsymbol{r})}{\psi^2}\right\}^2 \psi^2 = \psi^2 (\nabla_\perp \varphi - q_s \delta \mathbf{n}_\perp)^2. \tag{4.16}$$

When inserting the previous equations into (4.5), we obtain

$$\frac{1}{2\pi} \int_{\Omega_2} f_{\Omega_2} \ d\Omega = \tag{4.17}$$

$$= \frac{1}{2\pi} \int_{R-\delta}^{R} r' dr' \left\{ \frac{1}{2}(|\psi|^2 - 1)^2 + \frac{1}{2}(\boldsymbol{\tau}(\boldsymbol{r}))^2 + \left\{\frac{\boldsymbol{j}(\boldsymbol{r})}{\psi^2}\right\}^2 \psi^2 \right\}.$$

The integral over Ω_2 was calculated between $r = R$ and $r = R - \delta$, according to the exponential decay distance of the twist field. The last term of the energy expression (which is the analogy to the velocity of superconducting particles) decays as well exponentially from the boundary

$$\frac{j(\boldsymbol{r})}{|\psi|^2} = \frac{\delta}{R}(1 - \frac{\delta}{r})(l - \Phi_{LP})e^{-\frac{(R-r)}{\delta}}. \tag{4.18}$$

This expression agrees with (4.15) (see appendix A). It is only well defined in the edge region since it does not take in account currents in the bulk, according to the assumption that there is no influence between them and the edge currents.

The exponential decay of the current, according to figure (4.2) of the numerical calculations of equation (1.4), shows that this approximation is in good agreement for ψ that changes moderately in the edge region. Therefore it is correct to approximate the order parameter to an average value of $\psi = \psi_0 = constant$. It is then a matter of finding the proper value of the order parameter which minimizes the free energy. The integration of the twist term yields:

$$\frac{F_{twist}}{2\pi} = \frac{1}{4}\frac{\delta}{R}(\Phi_{LP} - \ell)^2 b \quad ; \quad b = 1 - e^{-2} - \frac{\delta}{2R} + \frac{3\delta}{2R}e^{-2}. \tag{4.19}$$

The integration of the first term of (4.17), that we shall denote as A yields:

$$\frac{A}{2\pi} = \frac{\delta}{2}(\psi_0^2 - 1)^2(R - \frac{1}{2}\delta). \tag{4.20}$$

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The velocity term is more difficult to calculate, it is obtained after we insert (4.18) into the integral:

$$\frac{F_{v_s}}{2\pi} = \psi_0^2(\ell-\Phi_{LP})^2 a \; ; \; a = \frac{\delta^3}{2R}[1-e^{-2}-\frac{5}{2}\frac{\delta}{R}+\frac{7}{2}\frac{\delta}{R}e^{-2}]+\frac{\delta^4}{R^2}\int_{R-\delta}^{R}\frac{e^{\frac{-2(R-r')}{\delta}}}{r'}d r'. \tag{4.21}$$

The radius of the system is $R \gg \delta$, so that the last integral in (4.21) becomes negligible. This term can however play a role for very small systems, when the edge region is of the size of the penetration depth. It is added that this term manifests the current dependence on the radius and δ which could suggest a strong connection between ψ_0 and δ. However for large R it is of second order and we shall consider them to be independent. The complete energy expression of the sample including the bulk then rewrites:

$$\frac{F_\ell(\Phi_{LP})}{2\pi} = \ell+\frac{\delta}{2}(\psi_0^2-1)^2(R-\frac{1}{2}\delta)+\frac{1}{4}\frac{\delta}{R}(\Phi_{LP}-\ell)^2 b+\psi_0^2(\ell-\Phi_{LP})^2 a \tag{4.22}$$

We wish to determine the value of ψ_0 through the minimization of the energy. The value we obtain is

$$\psi_0^2 = 1+\frac{a(\ell-\Phi_{LP})^2}{\delta(\frac{\delta}{2}-R)}. \tag{4.23}$$

It depends on a specific example of given system parameters. They are the applied twist field flux Φ_{LP} the value of the δ parameter (it is shown that although the δ parameter is not an external controlled parameter, there is a wide range of values for which the results are good), the size of the system and the number of dislocations. For the appropriate range of the system parameters, the value of ψ_0^2 was found to be larger than 0. (4.23) is inserted into (4.22). We obtain an expression for the free energy which is dependent only on Φ_{LP}, ℓ and the constants a an b which are functions of the δ parameter and the radius of the sample. The complete free energy contains the bulk and the edge energy expressions:

$$\frac{F_\ell(\Phi_{LP})}{2\pi} = \ell+c(\ell-\Phi_{LP})^2-d(\ell-\Phi_{LP})^4, \tag{4.24}$$

where $c = a+\frac{1}{4}\frac{\delta}{R}b$ and $d = \frac{a^2}{\delta(2R-\delta)}$. Equation (4.24) is the free energy that describes a mesoscopic cylinder of SmA which is inserted into a radial twist field. For $\delta \ll R$, d and c are positive parameters.

Chapter 5

Final results and conclusions

5.1 A selection mechanism (interpretation of the free energy functional)

We wish to analyze whether (4.24) shows that screw dislocations can be found inside the sample and when they are stable. It is also wished to obtain an exact number of screw dislocations that are induced at a given strength of a twist field.

The free energy of a sample of radius R and a penetration depth δ containing ℓ screw dislocations is a function of the applied twist flux Φ_{LP}.

If a certain value of the external twist field Φ_{LP} is applied, there is an energetically preferred number of screw dislocations that are induced into it. It is necessary to show that for a twist field that is not too large so as not to distroy the SmA phase, the free energy of a sample that does not contain any screw dislocations is larger than the free energy that contains at least one screw dislocation.

The smallest value of the twist field Φ_{LP} for the entrance of the first screw dislocation into the system corresponds to $\{F_{\ell=0} \leq F_{\ell=1}\} \mid_{\Phi_{LP}}$. Some numerical simulations for different system parameters have been done and presented in three figures.

Figure 5.1 presents energy surfaces for varying values of the δ parameter and the twist field surrounding the sample. It shows that a finite zone of system parameters and twist field values exists, in which the energy of the system that does not include a screw dislocation is larger than the energy of a system which includes a single screw dislocation.

In figure 5.2 the process of generating surfaces was repeated for different values of induced screw dislocations ℓ. A 'bird view' of the interception lines is presented.

The framework of this work sets a limit for the total number of allowed screw dislocations as a function of the size of the system.

The last figure (5.3) shows the results obtained for a single value of δ. The curves that appear denote the energy of the system, each for a different value of ℓ. They intercept at given values of the twist field. The lower envelope created by the intercepted curves represents the minimum value of the energy. We can see that it corresponds to a growing number of screw dislocations as the applied twist field grows.

These figures make it visible that for a finite area of the system parameter field there is a strong correlation between the number of screw dislocations and the external applied twist field. It is energetically preferred to insert additional screw dislocations into the system than repel them by screening currents. This is understood in the following way: For a certain applied twist stress the strain energy is lower if a dislocation is inserted into the center, enabling the boundary to relax. An opposite view would be that the twist flux can enter the system when the edge region vanishes and is located on the boundary. The bulk then is open to collect twist flux from the external field. As soon as an added dislocation enters the system, the bulk energy rises and it is preferred to shrink its size to enable a larger edge size that shields the entrance of further dislocations.

5.2   Conclusions

It has been shown that

1. For a mesoscopic system it is possible to use the de Gennes free energy to describe a system with only few screw dislocations.

2. A dual point is identified for which the free energy is topological and given by $F_{LG} = 2\pi\ell$.

3. The role of the boundary is to stabilize ℓ screw dislocations as a function of the applied external twist field.

4. Our study is the first analytical derivation towards the understanding of existence and stability of the TGB phase.

To summarize it, a closed expression of the free energy for a small SmA sample was obtained, from a direct derivation of the Landau-Ginzburg energy expression for liquid crystals. The derived energy expression contains as a parameter the number of screw dislocations that are induced into the system. It shows us that the minimization of the free energy allows to characterize a stable system that contains a finite number of screw dislocations.

5.3 A discussion on some questions

We have decided to mention some questions which have come up in the course of this work in form of a discussion.

- It looks as if the energy in equation (4.24) is unbounded and could even become negative. This is incorrect, since our theory is only valid when the value of Φ_{LP} is much smaller than πR and only for $R \gg \delta$. This will limit the number of screw dislocations in the system. As an example for the parameters $R = 10, \delta = 2.138$, like in figure (5.3), the twist flux allowed in the sample should be smaller than 5 (see Appendix B), and therefore the number of screw dislocations in the system will be equal or less than 3.

- Does our boundary condition disregard edge effects which are known to appear on finite SmA samples? More specifically, should the Rapini-Papoular form be added to an edge energy? Or is our theory not general or wrong without the Rapini-Papoular edge contribution? As we understand it, it is true that what we presented is in no way the most general case of a SmA sample and of the boundary conditions. However, we do believe that it is possible to generate an example in which the important physical parameters that influence the behavior of the system are those that we have included and analyzed in this work. Moreover, we also believe that this work is meaningful although it lacks generality and although it is probably not enough 'rounded up' to be implemented on an experiment. It is however a major step in that direction, since as a first approximation it identifies the most important parameters that influence such a system and it gives some principle results that characterize its physical properties.

- The use of the boundary condition (4.6) results from a physically reasonable assumption. However, it is not a result of physical properties, and one can rightfully claim that any result obtained depends on the specific boundary conditions that are set.

- Why does only the twist term in the expression of the free energy appear? This is actually the same question as the first one but somewhat more general. Again it is a matter of not addressing the most general situation, in which a SmA sample can be found. For a sample with a boundary we need to justify that it is possible to separate the effect of twist from the other terms of the Frank Oseen free energy. In general for a sample of infinite bulk this is obviously correct, since this is

exactly the meaning of the Frank Oseen free energy which is a manifestation of the diagonalization of the strain tensor of a sample. It is necessary to do some more research to determine how much this can be generalized for finite samples too. We have eluded this problem by setting very specific boundary conditions, including the way our sample is aligned proportionally to a stress field on it.

5.4   Suggestions for further research

In the following section some ideas that are out of the scope of this work, but can be followed on the basis of it, are mentioned.

- The analytical solution we presented is valid at the dual point. However, this is a point which is not reproducible in an experiment. For an experimental verification of the theory, it is necessary to show that the results we yielded are also valid in the vicinity of $\kappa = \frac{1}{\sqrt{2}}$.

- It would be also interesting to try and get the same results for a different boundary, like an infinite half space SmA.

- The numerical calculation showed that there are some interesting results as R gets smaller towards the size of Ω_1. It comes from the integral that was mentioned and dropped in 4.21.

- For a liquid crystal theory to be more complete, it is desirable to add the extra terms of Frank Oseen elastic energy considering also edge dislocations and other strains.
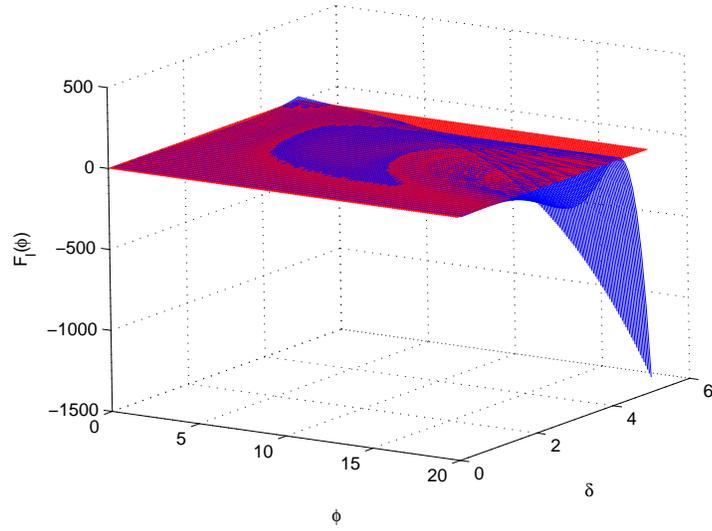
Figure 5.1: This figure is a numerical result of equation (4.24). The x axis is the twist field Φ_{LP}, the y axis is a varying penetration parameter δ value and the z axis is the corresponding value of the free energy. The sample radius chosen is 10 (dimensionless units). Each surface represents the energy of a sample that contains ℓ screw dislocations. Two surfaces are presented, the red surface is the zero energy plane F=0, the blue surface is the result of the deduction of a surface with a single screw dislocation $\ell = 1$ from a surface without one $\ell = 0$. A finite area of δ parameters and values of the twist field exist for which the blue surface lies above the zero energy plane.
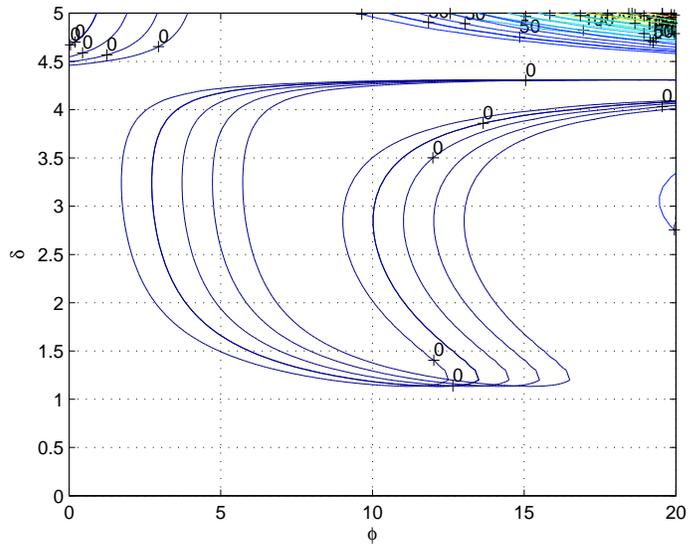
Figure 5.2: Presents a bird view of six surfaces, each contains a different number of screw dislocations. The contours are the interception lines between them. The contour that lies at the far left is the interception between surfaces of $\ell = 0$ and $\ell = 1$. Following to the right, the interception between $\ell = 1$ with $\ell = 2$ appears. This continues the same way as we move to the right, every contour that appears represents an additional dislocation in the system.
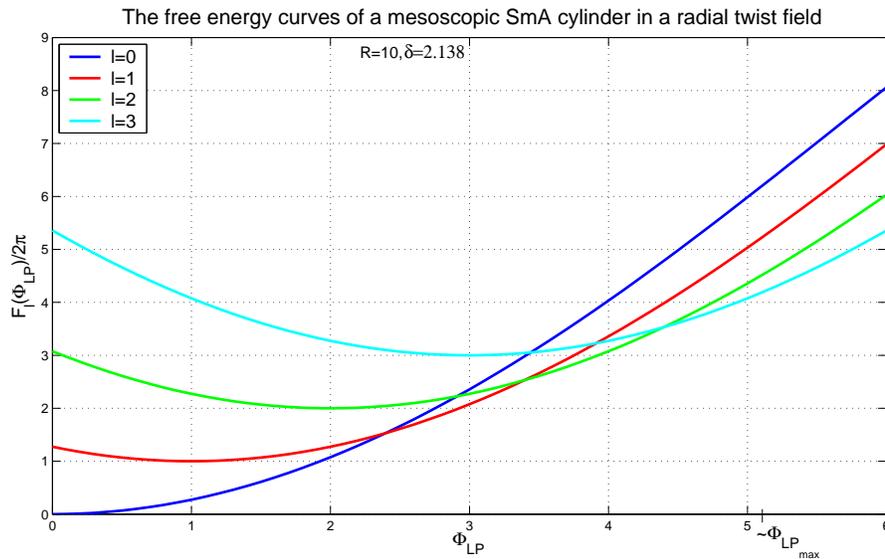
Figure 5.3: In this graph, each curve represents the energy of a system containing a different number of screw dislocations. The radius of the system is 10 and the value of δ is 2.138. The blue line represents the energy curve of a system that does not contain any dislocation. As we see, when the external twist field is small this curve corresponds to the lower envelope line and therefore to the minimum possible energy of the system. However, when the field grows the lowest energy corresponds to the red, the green and the light blue lines which correspond to a system that contains one, two and three screw screw dislocations.

Appendix A

Dependence of $|\psi|^2$ on δ

In deriving (4.18):

$$\frac{j(\boldsymbol{r})}{|\psi|^2} = \frac{\delta}{R}(1 - \frac{\delta}{\boldsymbol{r}})(l - \Phi_{LP})e^{-\frac{(R-\boldsymbol{r})}{\delta}},$$

we used (4.15):

$$\frac{\boldsymbol{\nabla} \times \boldsymbol{j}(\boldsymbol{r})}{|\psi|^2} = -\boldsymbol{\tau}(\boldsymbol{r}).$$

Using the assumption that ψ depends only weakly on δ when R is large, we shall prove that this is self consistent.

In (4.14) we obtained the following expression for the twist flux in the edge region:

$$\boldsymbol{\tau}(\boldsymbol{r}) = \frac{\Phi_{LP} - \ell}{R}e^{\frac{-(R-\boldsymbol{r})}{\delta}}\hat{z}$$

We can use the identity $\nabla \times \tau(r)\hat{z} = 2j\hat{\Theta}$ in order to derive the current density. We obtain $j = \frac{1}{2\delta}\frac{\ell - \Phi_{LP}}{R}e^{\frac{-(R-\boldsymbol{r})}{\delta}}$. If the last expression and (4.18) are valid, then they suggest the following dependence of the order parameter

$$|\psi|^2 = \frac{1}{2\delta^2(1 - \frac{\delta}{r})} \tag{A.1}$$

which is not independent on the penetration depth. However, this dependence is weak when R is large, since $\mathbf{r}$ will be much larger than δ and therefore (4.18) still agrees with (4.15). In order to show that, we insert the expression obtained for the order parameter into the current expression (4.18). When its curl is taken the following is obtained:

$$\frac{\boldsymbol{\nabla} \times \boldsymbol{j}(\boldsymbol{r})}{|\psi|^2} = -\boldsymbol{\tau}(\boldsymbol{r}) + \frac{\delta^2}{r^2}\boldsymbol{\tau}(\boldsymbol{r}). \tag{A.2}$$

For $\delta \ll r$ the term on the right is small and can be neglected, and we see that the assumption that ψ depends only weakly on δ is justified and self consistent.

Appendix B

An approximation of the twist flux allowed in a system of size R=10

The second assumption at the beginning of chapter 4 is $R \ll \frac{2\pi}{k_0}$ which is equivalent to $k_0 \ll \frac{2\pi}{R}$. If we insert this into equation (4.11) we obtain:

$$\Phi_{LP} = \frac{k_0 R^2}{2} \ll \pi R \tag{B.1}$$

Requiring that k_0 is smaller than $\frac{2\pi}{6R}$, amounts to assuming that the external twist field is such that in a cholesteric sample of the same size the director would have tilted by 60^0. In a SmA sample this is much less, we shall assume that it is not larger than 20^0, and therefore it is a small tilt. For a sample size $R = 10$, a good approximation for the maximum twist flux is:

$$\Phi_{LP} \leq \frac{1}{6}\pi 10 \simeq 5 \tag{B.2}$$

Figure (5.3) indicates that this corresponds to up to three dislocations in the system.

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בחלק השני של עבודה זאת נבחנה דוגמא של צילינדר אינסופי בעל רדיוס סופי שמצוי בתוך התחום שהוגדר כמסוסקופי. בתחום זה חישוב האנרגיה החופשית בנפרד עבור החלק פנימי של הצילינדר ובנפרד עבור תחום שפת הצילינדר הוא קירוב מוצדק.

מוצג כי החלק הפנימי הוא בעל אנרגיה המקורבת לאנרגיה הטופולוגית של Bogomoln'yi. אנרגיית השפה מתקבלת בחישוב של ביטוי האנרגיה החופשית הכללית כאשר תנאי שפה מתאימים מוגדרים.

בחרנו להשתמש בשיטת Little Parks לחישוב אנרגיית השפה. בהתאם לשיטה זאת השטף הכולל שעובר דרך הדגם אינו גבוהה מהשטף שעובר דרך אותו השטח לולא הדגם נמצא שם. לשם פשטות נעשה החישוב עבור שדה חיצוני בעל סימטריה צילינדרית ביחס למיקום הדגם, שכונה על ידנו שדה Little Parks.

תוצאת חישוב מראה שנוצר קשר בין מינימום האנרגיה הכללית של דגם חשוף לשדה בורגי חיצוני למספר ספציפי של SD בתוכו. ערכי השדה החיצוני עבורם המינימיזציה של אנרגיית המערכת כרוכה בהכנסת עיוות נוסף לתוך הדגם מוצגים.

תוצאה זו מצביעה על כך שכאשר למערכת יש רדיוס סופי מסוסקופי נוצר קשר בין המספר האבסולוטי של העיוותים בתוכה למינימום האנרגיה שלה.

התוצאות מוצגות בגרפים שבהם האנרגיה החופשית חושבה על ידי הצבת ערכים נומריים לרדיוס המערכת, חוזק השדה החיצוני ופרמטר δ.

כמו כן הוצג שישנו תחום שלם של ערכי הפרמטרים עבורם התוצאות שהתקבלו תקפות.

והסוג השני הינו פאזת Abrikosov שמאפשר את כניסתן של וורטקסים כך שנוצר שדה מגנטי בתוך על המוליך.

כאשר פרמטר Ginzburg $\kappa < \frac{1}{\sqrt{2}}$, על מוליך ישתייך לפאזת Meisner וכאשר $\kappa > \frac{1}{\sqrt{2}}$ הוא ישתייך לפאזת Abrikosov .

בכדי למצוא מהו מצב שיווי המשקל של על מוליך יש למצוא את המינימום של האנרגיה החופשית ביחס לפרמטר הסדר מחד וביחס לווקטור הפוטנציאל מאידך.
עבור ערך כללי של פרמטר Ginzburg חשבון וורייאציות מניב את שתי משוואות Landau ו Ginzburg. המשוואה הראשונה שמתקבלת היא עבור פרמטר הסדר והשנייה עבור ווקטור הפוטנציאל.
משוואות אלו אינן ליניאריות ומצב שיווי המשקל התרמודינמי שלהן אינו ידועה באופן כללי.
יוצא דופן יחיד מתקבל כאשר ערכו של פרמטר Ginzburg הוא בדיוק $\kappa = \frac{1}{\sqrt{2}}$ וכאשר המערכת הנדונה היא אפקטיבית דו מימדית ואינסופית, במצב זה ניתוח האנרגיה החופשית של Landau ו Ginzburg מניבה תוצאה מעניינת מאד.

עבור מערכת כזו ניתן למצוא מינימום לאנרגיה החופשית באופן אנליטי, מאחר שבמצב זה דרגת חופש אחת מתבטלת והאנרגיה החופשית ניתנת לניסוח מחדש באופן כזה שמתקבלות שני משוואות בשני נעלמים. אלו הן הזהויות של Bogomoln'yi.
זהויות אלו חשובות מאחר שאיחודם מוביל למשוואה פתירה עבור פרמטר הסדר. זוהי משוואת Liouville. משוואה זאת מאופיינת בכך שהפתרונות שלה מגדירים שדה שבתוכו ישנו מספר שלם של נקודות סינגולאריות.
מינימום האנרגיה החופשית שמתקבל במצב זה הוא הערך הטופולוגי $n2\pi$, כאשר n הינו מספר שלם.
משום כך n מתייחס למספר נקודות הסינגולאריות של פרמטר הסדר כלומר למספר הוורטקסים בתוך המערכת.
כלומר במצב שיווי המשקל האנרגיה מקבלת ערך טופולוגי שקשור למספר הוורטקסים במערכת.

יש להבחין בדקות אחת בעלת חשיבות, על סמך זהויות Bogomoln'yi לבדם עובדת קיומם של וורטקסים במערכת אינו מוכח. הזהויות אומנם מקשרות בין האנרגיה החופשית המינימלית למספר הוורטקסים במערכת, כך שהיא נוטה להימצא במצב שבוא האנרגיה הינה כפולה שלמה שלהם. אך בכך אין די בכדי לזהות מהו מספר הוורטקסים במערכת, והאם אלו כלל קיימים. מספר הוורטקסים נשאר פרמטר בלתי תלוי.

עבודה זאת נחלקה למעשה לשני חלקים, בחלק הראשון הוצגה אנליזה עבור דגם SmA בעל גוף צילינדרי שציר הסימטריה שלו אינסופי והרדיוס שלו גם אינסופי. צילינדר בעל ציר סימטריה אינסופי מהווה מערכת שבה שדה פרמטר הסדר הינו דו מימדי אפקטיבית, כאשר שדה הבורגיות החיצוני הוא בכיוון ציר הסימטריה.
במצב זה ניתן להשתמש באנלוגיה של de-Gennes ולהציג את האנרגיה החופשית לפי Bogomoln'yi כך שהאנרגיה המינימאלית שמתקבלת היא טופולוגית וקשורה למספר נקודות הסינגולאריות בתוך הצילינדר. סינגולאריות בפרמטר הסדר של SmA הינה עיוות בורגי (SD).
מאחר ש SmA הוא אנאיסוטרופי האנלוגיה מתקיימת רק כאשר הצפיפות והמספר של העיוותים הבורגיים במערכת מצומצם, ובכך ההתמקדות במסגרת עבודה זו.

תקציר

עבודת מחקר זאת מניחה את העקרונות התיאורטיים, בעזרת פיתוח אנליטי, לקיומם והופעתם
של עיוותים טופולוגיים מסוג Screw Dislocation (SD) בגבישים נוזליים שנמצאים בפאזת
Smectic A (SmA).

בנוסף מחקר זה גם מפרט ונותן דוגמה אחת עם תנאים ספציפיים שמאפשרים את היווצרותם
של עיוותים אלו. מוצג החישוב הנומרי שמבוסס על דוגמה זאת ותוצאותיו שכוללים את הופעתם
של עיוותים אלו.

שימושים קונקרטיים אפשריים לתוצאות עבודה זאת לא נדונו, והשימוש העיקרי הוא הבנתם של
הגורמים הפיזיקליים הבסיסים שמשפיעים על היווצרותם של העיוותים הטופולוגיים. אנו רואים
את תפקידה העיקרי של עבודה זאת בכך שהיא משמשת בסיס להמשך המחקר בנושאים
הקשורים לעיוותים טופולוגיים בכלל ו ל SD בפרט.

טרם פרסום עבודה זאת Lubensky ו Renn (1988) פרסמו את העבודה שהניחה את היסודות
לעבודתנו. במחקרם Lubensky ו Renn הציעו את קיומה של פאזה תיאורטית בשם
Twist Grain Boundary (TGB). זוהי פאזה של גרגירי SmA מסודרים כך שבין כל גרגיר
וגרגיר ישנה הפרדה על ידי חיץ מישורי שמורכב מסדרה מקבילה של SD.

בעבודתם Lubensky ו Renn הניחו כי עיוותים טופולוגיים מסוג SD קיימים ובהנחה זאת הראו,
שישנה כדאיות אנרגטית להיווצרותה של פאזת ה TGB, זאת כאשר מתקיימים עוד מספר
תנאים נוספים שאותם הם מפרטים.

ואכן כעבור שנה מפרסום מחקרם נמצאו עדויות ניסיוניות (Goodby 1989 ושות') שמצביעות
על קיומה של פאזת ה TGB. העיוותים הטופולוגיים מסוג SD שמופיעים בפאזה זאת מופיעים
במספר גדול ובלתי מוגבל.

מטרת מחקר זה הוא בהבנת סיבת קיומם הבסיסית של עיוותים טופולוגיים מסוג SD ותיאור
הופעתו של עיוות בודד או מספר מוגבל של עיוותים.

נקודת המוצא של עבודה זו הוא במחקרו של de-Gennes (1972) שהצביע על האנלוגיה
שקיימת בין מעבר הפאזה מוליך-לעל מוליך למעבר הפאזה nematic ל SmA. מעבר הפאזה
מוליך-על מוליך מתואר על ידי האנרגיה החופשית של Ginzburg ו Landau שבה מופיע
פרמטר סדר מרוכב לתיאור הפאזה העל מוליכה. במחקרו de-Gennes מראה כי גם פאזת
SmA בגבישים נוזליים ניתנת לתיאור על ידי פרמטר סדר מרוכב, ולכן מעבר הפאזה nematic
ל SmA מתוארת בעזרת האנרגיה החופשית של Ginzburg ו Landau.

האנלוגיה בין שני מעברי הפאזה הללו הינה רק בכך שישנה אנלוגיה באופי האנרגיות החופשיות
של פאזות אלו. אין כל קשר פיסיקלי אחר ברור בין על מוליכים ל SmA. במהותן אלו מערכות
פיסיקליות שאין ביניהם כל קשר, ולמרות זאת ניתן להסיק רבות מהאנלוגיה. ישנן מספר גדול
של תוצאות שהתקבלו במחקר על מעבר הפאזה בעל מוליכים שניתנות להמשלה עבור המחקר
של מעבר הפאזה בגבישים נוזליים.

את האנרגיה החופשית של Ginzburg ו Landau ניתן להציג בצורה חסרת מימד כך שהפרמטר
היחיד שבה היא תלויה הינו פרמטר חסר המימד א של Ginzburg. פרמטר זה תלוי רק
בתכונות הפנימיות של החומר ממנו עשוי על המוליך. אחת התוצאות שהתקבלו הוא כי ישנם שני
תחומי ערכים של פרמטר Ginzburg עבורם קיימים שני סוגים של על מוליכים שונים במהותם.
הסוג הראשון הקלאסי הוא פאזת Meisner שאינו מאפשר את כניסתן של וורטקסים לתוכו.

רשימת איורים

תוכן עניינים

מוקדש באהבה לאבי ד"ר אלכסנדר שטלהיים שמהווה עבורי דוגמה לחיקוי, ללא תמיכת הוריי לא הייתי מגיע עד הלום.
ובהערצה לאישתי מויקן שטלהיים שהעניקה לי את הכח ואת החוכמה להיתמודד עם כל הרגעים הקשים, ללא תמיכתה ואהבתה ספק עם הייתי מצליח.

ברצוני להודות לפרופ' סנקלפה גוש שהיה שותף חשוב לעבודה זו ועזר לי רבות בהבנה וליבון הנושאים הנדונים. כמו כן ברצוני להודות לריקי, מריה, אוהד וארי שהיו חברים ושותפים טובים לחדר ואנשי שיח טובים.

המחקר נעשה בהנחיית פרופ' אריק אקרמן בפקולטה לפיסיקה

עיוותים בורגיים במערכת מסוסקופית של גביש נוזל בפאזת

Smectic A

חיבור על מחקר

לשם מילוי חלקי של הדרישות לקבלת התואר

מגיסטר למדעים בפיסיקה

עמוס שטלהיים

הוגש לסנט הטכניון – מכון טכנולוגי לישראל