

A theory of superconducting ferroelectric heterostructures

weejoow hippe paper over gist enzo super vo

A. Heuvel



A theory of superconducting ferroelectric heterostructures

weejoow hippe paper over gist enzo super vo

by

A. Heuvel

to obtain the degree of Bachelor of Science
at the Delft University of Technology,
to be defended publicly on Monday January 1, 2024 at 10:00 AM.

Student number: 5619912
Project duration: September 2, 2024 – January 1, 2024
Thesis committee:
Prof. dr. M. Ali, TU Delft, supervisor TN faculty
Dr. P. Visser, TU Delft, supervisor EWI faculty
Prof. Dr. Y. Blanter, TU Delft, second supervisor TN faculty

This thesis is confidential and cannot be made public until December 31, 2024.

An electronic version of this thesis is available at <http://repository.tudelft.nl/>.



Preface

A preface...

*A. Heuvel
Delft, October 2024*

Abstract

A summary...

Contents

Preface	i
Abstract	ii
Nomenclature	iv
1 Introduction	1
2 Theory	2
2.1 Dielectric Materials	2
2.2 Superconductivity	2
2.2.1 Standard BCS Theory	2
2.3 Screening	3
3 1-Dimensional model	4
3.1 Setup	4
3.2 Limiting cases	4
3.3 Attractive interaction	4
3.4 Vector notation	5
3.5 Hamiltonian	6
3.6 Hamiltonian vector notation	7
3.7 Normal solution	7
3.8 Relative Coordinates	8
4 2-Dimensional model	10
5 Conclusion	11
References	12

Nomenclature

An overview of the units used, and common abbreviations and symbols

Defined Atomic Units

Symbol	Definition	Value in Atomic units	Value in SI units
\hbar	Reduced Planck constant	1	$1.054571\dots \times 10^{-34}$ Js
e^+	Elementary charge	1	$1.602176\dots \times 10^{-19}$ C
m_e	Electron rest mass	1	$9.109383\dots \times 10^{-31}$ kg
$4\pi\epsilon_0$	Vacuum permittivity	1	$1.112650\dots \times 10^{-10}$ Fm ⁻¹

Derived Atomic Units

Symbol	Definition	Value in Atomic units	Value in SI units
a_0	Bohr radius	$4\pi\epsilon_0\hbar^2/m_e(e^+)^2 = 1$	$5.291772\dots \times 10^{-11}$ m
E_h	Hartree energy	$\hbar^2/m_e a_0^2 = 1$	$4.359744\dots \times 10^{-18}$ J
e^-	Electron charge	$-e^+ = -1$	$1.602176\dots \times 10^{-19}$ C

Abbreviations

Abbreviation	Definition
ISA	International Standard Atmosphere
...	

Symbols

Symbol	Definition	Unit
V	Velocity	[m/s]
...		
ρ	Density	[kg/m ³]
...		

1

Introduction

An introduction... [3]

2

Theory

2.1. Dielectric Materials

Dielectric materials, or dielectrics, are materials that are polarized by the presence of an electric field. There are two types of dielectrics. One type polarizes in the direction of the electric field, the other opposite to it. In this study, we assume a dielectric which polarizes in the direction of the electric field. Dielectrics consist of a bunch of dipoles arranged periodically, as can be seen in figure 2.1

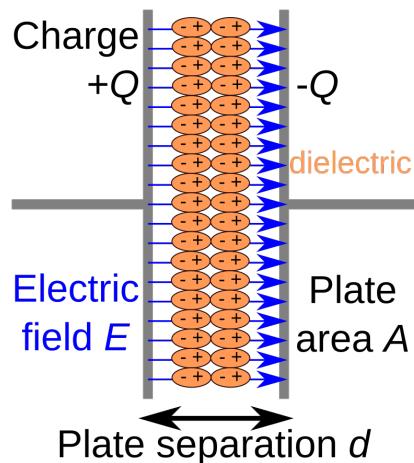


Figure 2.1: Schematic representation of a dielectric. The external electric field polarizes the material causing dipoles to point opposite to the electric field

2.2. Superconductivity

There are two types of superconductors. Conventional ones, and unconventional ones. The standard theory of superconductivity, named BCS theory after Bardeen, Cooper, and Schrieffer, uses the same basic principles to explain superconductivity as more advanced models. These principles are also a key part of describing ferroelectric superconducting heterostructures. In BCS theory, it is shown that under the right conditions, two electrons can form bound pairs at an energy below the Fermi level.

2.2.1. Standard BCS Theory

In standard BCS theory, the conditions for forming bound pairs of electrons are as follows. The two electrons are assumed to be in a free electrons, added to a Fermi sea at a temperature of 0K. These electrons interact with eachother, through both an electric repulsion from a screened Coulomb interaction, and another interaction mediated by phonons. The phonon-mediated interaction here is key. Scattering of one of the electrons from a momentum \mathbf{k} to a momentum \mathbf{k}' . This creates a phonon of

momentum $\mathbf{k} - \mathbf{k}' = \mathbf{q}$, that is carried through the atom core ions in the material. This process is shown schematically in figure 2.2 .

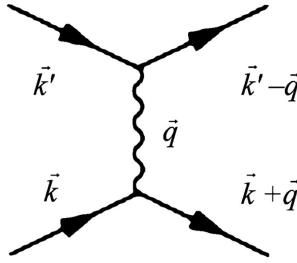


Figure 2.2: Schematic representation of electron-electron interaction mediated by a phonon with momentum $\mathbf{q} = \mathbf{k} - \mathbf{k}'$

It is shown by de Gennes [2] using the so-called "jellium model" that this gives rise to an effective attractive interaction between the two electrons given by

$$V(\mathbf{q}, \omega) = \frac{4\pi(e^+)^2}{q^2 + k_s^2} \left(1 + \frac{\omega_q^2}{\omega^2 - \omega_q^2} \right) \quad (2.1)$$

Where $\frac{1}{k_s}$ is the screening length, also known as the screening constant κ , ω_q is the characteristic frequency of the phonon, and ω is the characteristic frequency of the electrons, defined by $\hbar\omega = \xi_{\mathbf{k}'} = \xi_{\mathbf{k}}$, with $\xi_{\mathbf{k}}$ being the energy of the electron with momentum \mathbf{k} .

2.3. Screening

In conductors, electric fields behave differently to in a vacuum. The presence of positively charged ions and negatively charged electrons cause electric potentials to drop exponentially with distance. Using the Thomas-Fermi approximation [1], we find a dielectric function,

$$\epsilon(r) = \epsilon_0 e^{\kappa r} \quad (2.2)$$

Where κ is the so-called screening constant. Or in other words, all electric potentials are multiplied by an $e^{\kappa r}$ term.

3

1-Dimensional model

3.1. Setup

We consider a system of two interacting quantum-mechanical electrons and a classical dipole. We take the electrons on the x-axis, a fixed distance h apart from the dipole. Further, we assume a strong and constant electric field E_0 at an angle θ_0 to the x-axis. The dipole has a dipole moment of d , pointing in the direction of the total electric field, that being the sum of the external electric field and the electric field caused by the two electrons. It is further assumed all electric fields are screened, with a screening constant κ . This setup is shown in figure 3.1.

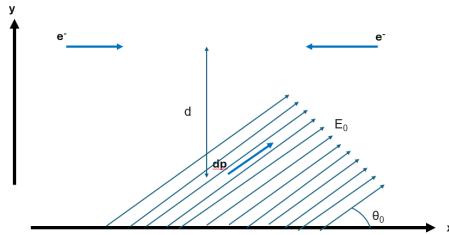


Figure 3.1: Setup of the system. The dipole is at the origin, with the electrons at a distance h from the dipole. The external electric field is at an angle θ_0 to the x-axis.

3.2. Limiting cases

To check the physical validity of a model, it is important to test for extreme values of parameters in a model, and see if they make intuitive and physical sense.

3.3. Attractive interaction

The repulsive interaction between electrons due to Coulomb interaction is given by the potential energy $V_C(x_1, x_2) = \frac{e^2}{4\pi\epsilon_0|x_1-x_2|}$. Taking the screening from ions into account we find $V_C(x_1, x_2) = \frac{e^2}{4\pi\epsilon_0|x_1-x_2|} e^{-\kappa|x_1-x_2|}$

The dipole is polarized by the presence of an external electric field. The electric field E_0 is given by:

$$\mathbf{E}_0 = E_0(\cos(\theta_0)\hat{x} + \sin(\theta_0)\hat{y}) \quad (3.1)$$

Where E_0 is the magnitude of the electric field, and θ_0 is the angle of the electric field to the x-axis.

The electric field due to an electron at the location of the dipole is given by:

$$\mathbf{E}_{e1} = \frac{e^-}{4\pi\epsilon_0(x_1^2 + d^2)} \hat{r} \quad (3.2)$$

Where \hat{r} is the unit vector pointing from the dipole to the electron, given by $\frac{x_1}{\sqrt{x_1^2 + d^2}} \hat{x} + \frac{d}{\sqrt{x_1^2 + d^2}} \hat{y}$, and similar for x_2 . This gives a total electric field at the dipole of

$$\mathbf{E}_{tot} = \begin{pmatrix} \cos(\theta_0)E_0 + \frac{e^-}{4\pi\epsilon_0} \left(\frac{x_1}{(x_1^2 + d^2)^{3/2}} + \frac{x_2}{(x_2^2 + d^2)^{3/2}} \right) \\ \sin(\theta_0)E_0 + \frac{e^-}{4\pi\epsilon_0} \left(\frac{d}{(x_1^2 + d^2)^{3/2}} + \frac{d}{(x_2^2 + d^2)^{3/2}} \right) \end{pmatrix} \quad (3.3)$$

Since the dipole will try to align with the electric field, we find that the angle the dipole will make with the x-axis will be given by $\arctan \dots, \dots$. By taking a taylor approximation of $\arctan(x)$, we find

$$\arctan(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} x^{2n+1} \quad (3.4)$$

Which we approximate with $\arctan(x) \approx x$. Further, using $\cos(\theta_0)E_0 \gg \frac{e^-}{4\pi\epsilon_0}$, and using a Taylor approximation to find $\frac{d}{(x^2 + d^2)^{3/2}} \approx \frac{1}{d^2} - \frac{3x^2}{2d^4}$. This leads to the following equation for θ

$$\theta = \frac{\sin(\theta_0)E_0 + \frac{e^-}{4\pi\epsilon_0} \left(\frac{2}{d^2} - \frac{3(x_1^2 + x_2^2)}{2d^4} \right)}{\cos(\theta_0)E_0} \quad (3.5)$$

We will expand $\arctan(x)$ around $x = \tan(\theta_0)$. Using $\frac{d}{dx} \arctan(x) = \frac{1}{1+x^2}$ and $\frac{d^2}{dx^2} \arctan(x) = \frac{-2x}{(1+x^2)^2}$, we find the second order approximation of $\arctan(x)$ around $x = \tan(\theta_0)$ to be $\arctan(x) \approx \theta_0 + \frac{x - \tan(\theta_0)}{1 + \tan(\theta_0)^2} - \frac{\tan(\theta_0)(x - \tan(\theta_0))^2}{(1 + \tan(\theta_0)^2)^2}$. From here, we disregard any terms higher than second order. This gets us

Using small angle approximations for $\sin(\theta)$ and $\cos(\theta)$

3.4. Vector notation

Doing the same calculations using vector notation, we find the following. First, we have

$$\mathbf{E}_0 = \begin{pmatrix} E_0 \cos(\theta_0) \\ E_0 \sin(\theta_0) \end{pmatrix} \quad (3.6)$$

Assuming a screened electric field, we take the Yukawa potential

$$V_\kappa(\mathbf{r}_i) = \frac{(e^-)^2}{4\pi\epsilon_0 r_i} e^{-\kappa r_i} \quad (3.7)$$

Where κ is the screening constant, r is the distance between the electron and the dipole, and \mathbf{r} is the vector pointing from the dipole to the electron. We want to know the electric field at the dipole. The electric field at the dipole due to an electron at position \mathbf{r}_i

$$\mathbf{E} = -\nabla V_\kappa(\mathbf{r}_i) = \frac{(e^-)^2}{4\pi\epsilon_0} \frac{e^{-\kappa r_i}}{r_i} \left(\kappa + \frac{1}{r_i} \right) \hat{r}_i \quad (3.8)$$

This would mean the dipole would point in the direction

$$\hat{d} = \hat{E} = (\mathbf{E}_0 + \mathbf{E}_1 + \mathbf{E}_2) / |\mathbf{E}_0 + \mathbf{E}_1 + \mathbf{E}_2| \quad (3.9)$$

Where \mathbf{E}_0 is the externally applied electric field, \mathbf{E}_1 is the electric field due to the first electron, and \mathbf{E}_2 is the electric field due to the second electron. That gives a dipole moment of

$$\mathbf{d} = d\hat{\mathbf{d}} \quad (3.10)$$

Then the potential energy of the electrons due to the dipole is given by

$$V_{dp,i} = \frac{\mathbf{d} \cdot \mathbf{r}_i}{4\pi\epsilon_0|\mathbf{r}_i|^3} \quad (3.11)$$

Including screening we find

$$V_{dp,i} = \frac{\mathbf{d} \cdot \mathbf{r}_i}{4\pi\epsilon_0|\mathbf{r}_i|^3} e^{-\kappa|\mathbf{r}_i|} \quad (3.12)$$

Further, we have the interaction between the two electrons, given by

$$V_C = \frac{e^-}{4\pi\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} \quad (3.13)$$

Adding screening, we get

$$V_C = \frac{e^-}{4\pi\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} e^{-\kappa|\mathbf{r}_1 - \mathbf{r}_2|} \quad (3.14)$$

3.5. Hamiltonian

When using the single dipole model, the Hamiltonian of the system consists of six parts and is give by:
This hamiltonian is given by $\hat{H} = \hat{H}_{e_1} + \hat{H}_{e_2} + \hat{H}_{e_1,e_2} + \hat{H}_{e_1,dip} + \hat{H}_{e_2,dip} + \hat{H}_{e_1,F} + \hat{H}_{e_2,F}$

Where the terms are kinetic energy of electron 1, the kinetic energy of electron 2, the kinetic energy of the dipole, the interaction between the two electrons, the interaction between electron 1 and the dipole, and the interaction between electron 2 and the dipole respectively.

The kinetic energy for the electron in one dimension is given by $\hat{H}_{e_1} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2}$ and $\hat{H}_{e_2} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2}$

Where x_1 and x_2 are the position of electron 1 and electron 2 respectively. The kinetic energy for the dipole is given by $\hat{H}_{dp} = -\frac{\hbar^2}{2I} \frac{\partial^2}{\partial \theta^2}$

The interaction between the two electrons is given by $\hat{H}_{e_1,e_2} = V_C(x_1, x_2)$

The interaction between electron 1 and the dipole is given by $\hat{H}_{e_1,dip} = \frac{pqe^-}{4\pi\epsilon_0(x_1^2 + d^2)^{3/2}}(x_1 \cos(\theta) + d \sin(\theta))$

The interaction between electron 2 and the dipole is given by $\hat{H}_{e_2,dip} = \frac{p \cos(\theta)}{4\pi\epsilon_0 x_2^2}$

The interaction between electron 1 and the external electric field is given by $\hat{H}_{e_1,F} = -eE_0 \cos(\theta)$

The interaction between electron 2 and the external electric field is given by $\hat{H}_{e_2,F} = -eE_0 \cos(\theta)$

These two terms will given a constant offset energy, and are therefore not relevant.

Finally, the interaction between the dipole and the external electric field is given by $\hat{H}_{dp,F} = -pE_0 \cos(\theta - \theta_0)$, where θ_0 is the angle the external electric field makes with the x-axis.

Now the goal is to find a state with an energy $\langle \psi(x_1, x_2, \theta) | \hat{H} | \psi(x_1, x_2, \theta) \rangle < E_F$

The fermi energy is the energy of the

So first of all, one electron needs to be closer to the dipole than the other, to cause a rotation in the dipole. So we know the dipole is in a state rotated towards, say, positive x. Then electron 1, to the left of the dipole, is it a reasonably large distance from the dipole. Electron 2, to the right of the dipole, is at a reasonably small distance from the dipole. So let's say they're all Gaussian, with θ centered at $\pi/4$, x_1 at a distance of -1, and x_2 at a distance of 0.5.

Let's fill this into the Hamiltonian, and not worry about complex coefficients or normalization for now?

3.6. Hamiltonian vector notation

Now that we have the interaction between electrons mediated by the dipole, we can give the Hamiltonian of the system. This Hamiltonian consists of five parts: The kinetic energies of each electron, the interaction of the electrons through the Coulomb force, the interaction mediated by the dipole, and the interaction with the external electric field. This leads to a Hamiltonian $\hat{H} = \hat{H}_{e_1} + \hat{H}_{e_2} + \hat{H}_C + \hat{H}_{dp} + \hat{H}_E$. Where the terms are the kinetic energy of each electron, the Coulomb interaction, the dipole mediated interaction, and the external electric field interaction respectively.

3.7. Normal solution

Now let's try find a state with negative energy. Due to the coulomb interaction between electrons, unentangled electrons do not give a convergent solution. Therefore, we try the entangled state $\psi(x_1, x_2) = e^{\frac{-(x_1-a_1)^2-(x_2-a_2)^2}{b}}(x_1 - x_2)$ with normalization constant $\frac{\pi}{4}b(2(a_1 - a_2)^2 + b)$. $|\psi(x_1, x_2)|^2$ is shown in figure 3.2

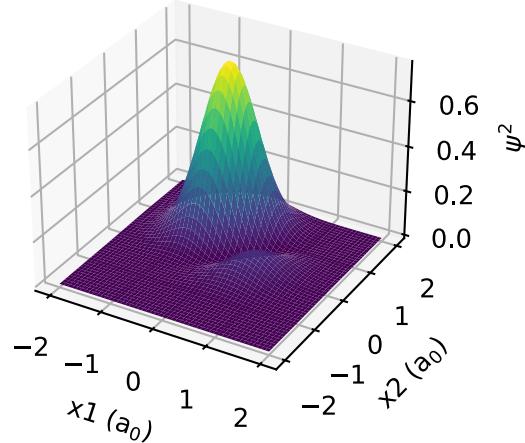


Figure 3.2: Schematic representation of electron-electron interaction mediated by a phonon with momentum $\mathbf{q} = \mathbf{k} - \mathbf{k}'$

To calculate the kinetic energy terms, we want to take the Fourier transform of the wavefunction. To transform $\psi(x_1, x_2)$ into a function of momenta, $\phi(p_1, p_2)$, we use

$$\mathcal{F}\{\psi(x_1, x_2)\}(p_1, p_2) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi(x_1, x_2) e^{\frac{-i}{\hbar}(p_1 x_1 + p_2 x_2)} dx_1 dx_2 \quad (3.15)$$

Where $p_i = \hbar k_i$ is the quantum mechanical momentum. This gives us

$$\begin{aligned}\phi(p_1, p_2) &= \int_{-\infty}^{\infty} x_1 e^{-\frac{1}{b}x_1^2 + (\frac{2a_1}{b} - \frac{ip_1}{\hbar})x_1 - \frac{a_1^2}{b}} dx_1 \int_{-\infty}^{\infty} e^{-\frac{1}{b}x_2^2 + (\frac{2a_2}{b} - \frac{ip_2}{\hbar})x_2 - \frac{a_2^2}{b}} dx_2 \\ &\quad - \int_{-\infty}^{\infty} x_2 e^{-\frac{1}{b}x_2^2 + (\frac{2a_2}{b} - \frac{ip_2}{\hbar})x_2 - \frac{a_2^2}{b}} dx_2 \int_{-\infty}^{\infty} e^{-\frac{1}{b}x_1^2 + (\frac{2a_1}{b} - \frac{ip_1}{\hbar})x_1 - \frac{a_1^2}{b}} dx_1\end{aligned}\quad (3.16)$$

Which evaluates to

$$\phi(p_1, p_2) = \left(\frac{-a_1}{b} + \frac{ip_1}{2\hbar} + \frac{a_2}{b} - \frac{ip_2}{2\hbar} \right) \pi b^2 e^{-\frac{a_1^2}{b} + (\frac{a_1}{2\sqrt{b}} - \frac{i\sqrt{b}p_1}{2\hbar})^2} e^{-\frac{a_2^2}{b} + (\frac{a_2}{2\sqrt{b}} - \frac{i\sqrt{b}p_2}{2\hbar})^2} \quad (3.17)$$

Now, to use this to calculate the potential energy, we need to take it times its conjugate. We find

$$|\phi(p_1, p_2)|^2 = \pi^2 b^4 \left(\frac{(a_2 - a_1)^2}{b} + \frac{(p_1 - p_2)^2}{4\hbar^2} \right) e^{-\frac{a_1^2}{2b} - \frac{bp_1^2}{2\hbar^2}} e^{-\frac{a_2^2}{2b} - \frac{bp_2^2}{2\hbar^2}} \quad (3.18)$$

3.8. Relative Coordinates

It can be useful to describe systems using different coordinates. To this end, we introduce the relative coordinate system. Here, we define $r = r_2 - r_1$ and $R = \frac{r_1 + r_2}{2}$. With this transformation, we also get new momentum coordinates. Defining $q = -i\hbar \frac{\partial}{\partial r}$ and $p = -i\hbar \frac{\partial}{\partial R}$, we find $q = \frac{p_1 - p_2}{2}$ and $p = p_1 + p_2$, where $p_1 = -i\hbar \frac{\partial}{\partial r_1}$ and $p_2 = -i\hbar \frac{\partial}{\partial r_2}$.

This gives us interaction terms as follows:

With the wavefunction $\phi(r, R) = e^{\frac{-2}{b}(R - \frac{1}{2}(a_1 + a_2))^2 + \frac{-1}{2b}(r + (a_1 - a_2))^2 + \frac{-1}{b}(a_1 + a_2)^2} r$ Which becomes seperable into $f(r)g(R) = e^{\frac{-1}{2b}(r + (a_1 - a_2))^2} r e^{\frac{-2}{b}(R - \frac{1}{2}(a_1 + a_2))^2}$ With normalization constant $\frac{1}{2}(2(a_2 - a_1)^2 + b)\sqrt{\pi b}$ for $f(r)$ and normalization constant $\frac{\sqrt{b}\pi}{2}$ for $g(R)$ Relative coordinates also change the interaction terms: $V_C = \frac{e^-}{4\pi\epsilon_0 r} e^{-\kappa r}$ We get $\hat{d} = \mathbf{E}_0 + \mathbf{E}_1 + \mathbf{E}_2$ Which results in a wavefunction looking like figure 3.3

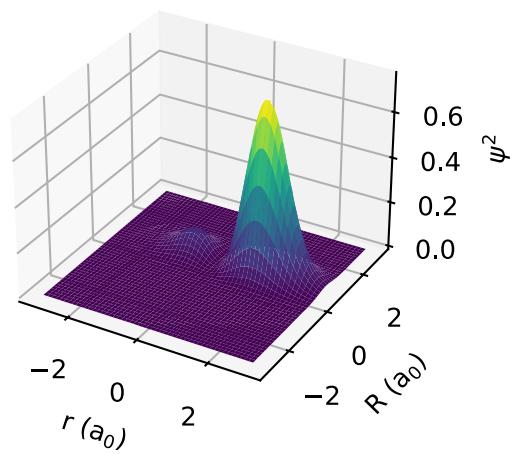


Figure 3.3: Trial wavefunction ψ in relative coordinates

4

2-Dimensional model

1-dimensional models, while easy to work with, do not always give a correct physical description. We expand on the 1-dimensional model by allowing electrons to move both in the x and y direction. Later, we will expand to a model where the electrons can also move in the positive z direction.

Since we have already been using vector notation, adding another dimension won't prove very difficult. Following the same steps as in section 3.4, we take an external electric field

$$\mathbf{E}_{\text{ext}} = \begin{pmatrix} E_{\text{ext}} \sin(\theta_{\text{ext}}) \cos \phi_{\text{ext}} \\ E_{\text{ext}} \sin(\theta_{\text{ext}}) \sin \phi_{\text{ext}} \\ E_{\text{ext}} \cos(\theta_{\text{ext}}) \end{pmatrix} \quad (4.1)$$

5

Conclusion

A conclusion...

References

- [1] N.W. Ashcroft and N.D. Mermin. *Solid state physics*. 2003.
- [2] P.G. de Gennes. *Superconductivity in metals and alloys*. 1st ed. Westview press, 1966.
- [3] I. Surname, I. Surname, and I. Surname. "The Title of the Article". In: *The Title of the Journal* 1.2 (2000), pp. 123–456.