

Rationalization Questions in Particle Physics

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ZUSAMMENFASSUNG

Theoretische Vorhersagen in der Hochenergie-Teilchenphysik erfordern die Berechnung von Feynman-Integralen. Im Zuge solcher Berechnungen treten in bestimmten Zwischenschritten oft Quadratwurzeln in den kinematischen Variablen auf. Eine Möglichkeit, Feynman-Integrale in Form multipler Polylogarithmen darzustellen, besteht darin, alle auftretenden Quadratwurzeln durch eine geeignete Variablentransformation zu rationalisieren. Diese Strategie lässt sich auf sehr viele Berechnungen der modernen Hochenergiephysik anwenden. In dieser Arbeit untersuchen wir daher die Frage, mit welchen Methoden man Quadratwurzeln rationalisieren kann. Einerseits werden wir feststellen, dass nicht alle Quadratwurzeln rationalisierbar sind. Für diese Fälle erarbeiten wir Kriterien, die es uns erlauben werden, die Nicht-Rationalisierbarkeit einer gegebenen Quadratwurzel zu beweisen. In vielen anderen Berechnungen ist eine Rationalisierung der auftretenden Quadratwurzeln jedoch durchaus möglich. Für die Behandlung solcher Fälle werden wir einen Rationalisierungsalgorithmus erarbeiten. Dieser ist immer dann anwendbar, wenn die gegebene Quadratwurzel einer Hyperfläche entspricht, die einen Punkt der Multiplizität $d - 1$ aufweist, wobei d den Grad der Hyperfläche beschreibt. In diesem Zusammenhang werden wir außerdem den F -Zerlegungssatz formulieren. Dieser erlaubt es uns, den Rationalisierungsalgorithmus auch auf viele andere Quadratwurzeln anwenden zu können, deren assoziierte Hyperfläche keinen Punkt der Multiplizität $d - 1$ aufweist. Abschließend präsentieren wir das Softwarepaket **RationalizeRoots**, das die von uns untersuchten Rationalisierungsmethoden für **Mathematica** und **Maple** implementiert. Alle hier diskutierten Techniken werden wir anhand von Beispielen aus der modernen Hochenergiephysik erklären und verdeutlichen.

ABSTRACT

Theoretical predictions in high energy particle physics require the computation of Feynman integrals. Certain steps in these computations generate square roots in the kinematic variables. One way to express Feynman integrals in terms of multiple polylogarithms is to rationalize all occurring square roots by a suitable variable change. Although such a variable change does not always exist, there are many examples from recent high energy physics that admit a rationalization. In this thesis, we study the question of how to rationalize a given set of square roots in detail. On the one hand, not all square roots are rationalizable. For these cases, we establish criteria that allow us to prove non-rationalizability in a rigorous manner. On the other hand, many square roots admit a rationalization. For these cases, we give a rationalization algorithm that is applicable whenever the hypersurface associated to the square root has a point of multiplicity $d - 1$, where d is the degree of the hypersurface. Furthermore, we present the F -decomposition theorem, which expands the scope of the algorithm to square roots whose rationalization would otherwise be out of reach. Lastly, we present the `RationalizeRoots` software package, which implements our rationalization methods for `Mathematica` and `Maple`. We clarify all of our techniques through several examples from modern high energy physics.

PREFACE

At the time when I attended my very first physics conference and asked one of the senior scientists how to write a good piece in mathematical physics, I got the following answer:

“Marco,” he said, “whenever you explain algebraic geometry to physicists, the odds are high that none of them has ever read about anything in the field. Thus, you should not hesitate to introduce even the most basic notions and only raise the abstraction level if you absolutely have to. Keep in mind that your readers are looking for a text that solves their problems, not for a text that lowers their academic egos.”

I fully agree. Writing a thesis in such a way does, however, come with some trade-offs in mathematical generality and conciseness. Mathematicians should, therefore, bear in mind that this text is deliberately written to be accessible for theoretical physicists.

Most of the material is based on [1]–[3]. In addition, I also included not yet published insights from [4].

It is my sincere hope that the presented material will serve as a useful resource for many physicists and will inspire other algebraic geometers to build upon the results of this thesis.

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Introduction

High energy particle physics studies the fundamental building blocks of nature: elementary particles and their interactions. It assumes that all interactions of matter are governed by four fundamental forces:

1. Gravity
2. Electromagnetic interaction
3. Weak interaction
4. Strong interaction

We experience the effects of gravity and electromagnetism in our everyday life. Strong and weak interactions, however, are only present at subatomic scales.

There are two theoretical frameworks to investigate these fundamental forces: Einstein's general relativity for gravity and the Standard Model (SM) of particle physics for electromagnetic, weak, and strong interactions. While general relativity is an active field of research in and of itself, much effort in contemporary particle physics is devoted to the investigation of the SM.

To test the validity of the SM, physicists study scattering processes, i.e., they collide particles at high energies in huge particle colliders—the world's most famous being the Large Hadron Collider (LHC) at the CERN laboratory in Geneva, Switzerland. The advancing precision of the experimental measurements requires equally precise theoretical predictions. To perform the necessary computations, one has to solve Feynman integrals. These integrals are often expressible in terms of special functions, called multiple polylogarithms (MPLs), which admit a representation as iterated integrals with integration kernels of the form

$$\frac{dx}{x-z},$$

where z is independent of x but may depend on kinematic variables such as particle masses or momenta. In practice, however, one often encounters integration kernels that involve square roots, for example,

$$\frac{dx}{\sqrt{(x - z_1)(x - z_2)}}.$$

In order to find a result in terms of MPLs, one can try to rationalize the square roots in the integration kernels by a suitable variable change and, subsequently, apply partial fractioning to express the integral in terms of the desired integration kernels plus trivial integrations.

With this technique, one can solve a large number of Feynman integrals in terms of MPLs. For this reason, the problem of rationalizing a given set of square roots has played a crucial role in modern physics applications [5]–[16]. It is tempting to think that the rationalization of square roots is the only way to express the solution in terms of MPLs. Let us, therefore, emphasize that Heller, Schabinger, and von Manteuffel recently discovered the first examples of Feynman integrals expressible through MPLs despite the presence of non-rationalizable square roots [13]. Nevertheless, the rationalization of square roots is often the most convenient strategy to find a solution in terms of MPLs.

This thesis provides a thorough study of rationalization methods for square roots. Part 1 covers the foundations that are necessary to understand the physical background and to get acquainted with the mathematical tools. Further, it gives a brief historical overview, showing that the rationalization question is one of the oldest problems in mathematics. In Part 2, we will establish specific criteria that help us decide whether a rationalization of a given set of square roots is possible. Finally, Part 3 gives a detailed account on practical rationalization techniques such as our main algorithm, the *F*-decomposition theorem, and the usage of the `RationalizeRoots` package [1].

Part 1

Foundations

CHAPTER 1

The Rationality Question in Mathematics

The following chapter covers some of the fundamental results about the rationality of algebraic hypersurfaces. Its purpose is to, on the one hand, provide the reader with an overview of the most important mathematical results on the topic and, on the other hand, give credit to the outstanding mathematicians that developed those results.

1.1. CURVES AND CALCULUS: A BRIEF HISTORY

In his “Géométrie” [17] from 1637, Descartes showed that conical sections can be viewed as zero sets of degree-2 polynomials. A few decades later, in the last quarter of the same century, Leibniz and Newton developed the foundations of differential and integral calculus. This triggered one of most fundamental mathematical questions: If $f(x)$ is a *function*—a term coined by Leibniz—how can one explicitly integrate differentials of the form $f(x)dx$?

For *rational* functions, a solution to this problem is known since the time of Euler: using partial fraction decomposition, one can write the primitive

$$\int R(t) dt$$

of a rational function $R(t)$ as a sum of logarithms plus a rational function. For example, one may express the arctangent function through a logarithm via

$$\int_0^z \frac{dt}{1+t^2} = \frac{1}{2} \int_0^z \left(\frac{dt}{1+it} + \frac{dt}{1-it} \right) = \frac{1}{2i} \log \left(\frac{1+iz}{1-iz} \right).$$

During this era, the concerted efforts of Bernoulli, Fagano, Legendre, Euler, and Abel culminated in the study of *abelian integrals*, i.e., primitives of the form

$$\int R(x, y) \, dx,$$

where $R(x, y)$ is a rational function depending on two variables that are related through a polynomial equation

$$f(x, y) = 0.$$

Thus, one may say that the given integral “depends” on the curve defined by this polynomial. For example, we may say that the integral

$$\int \frac{x + \sqrt{1 - x^2}}{x^2 + \sqrt{1 - x^2}} \, dx$$

“depends on the circle” since we can view it as an integral

$$\int \frac{x + y}{x^2 + y} \, dx$$

of a rational function in two variables that are related through the polynomial equation

$$x^2 + y^2 - 1 = 0.$$

This raised the following question: Under which conditions can an abelian integral be reduced to the primitive of a rational function and, therefore, be computed as a sum of logarithms plus a rational function? As we will see in the upcoming section, this naturally leads us to the question under which conditions a given algebraic curve is parametrizable by rational functions.

1.2. THE RATIONALITY QUESTION FOR CURVES

Before we proceed with the discussion on abelian integrals, let us give a brief introduction to rational algebraic curves.

We define an *affine plane curve* as the curve consisting of the points of \mathbb{C}^2 whose coordinates x, y satisfy an equation

$$f(x, y) = 0,$$

where f is a non-constant polynomial with complex coefficients. A curve is called *irreducible* if its defining polynomial is irreducible over the field of complex numbers. The *degree* of the curve is defined as the degree of f .

An irreducible affine plane curve C defined by $f(x, y) = 0$ is called *uni-rational* or *parametrizable by rational functions* if there exist two rational functions $\phi_x(t), \phi_y(t) \in \mathbb{C}(t)$, at least one non-constant, such that

$$f(\phi_x(t), \phi_y(t)) = 0$$

as an identity in the complex variable t . Notice that, if $t = t_0$ is a fixed value and not one of the finitely many values at which the denominator of $\phi_x(t)$ or $\phi_y(t)$ vanishes, then $(\phi_x(t_0), \phi_y(t_0))$ is a point of C .

We say that C is *rational* if there is a rational parametrization $(\phi_x(t), \phi_y(t))$ such that the map $t \mapsto (\phi_x(t), \phi_y(t))$ is a one-to-one correspondence between the values of t and the points of C , provided that we exclude certain finite sets from both the set of values of t and the points of C . A map with this property is called a *birational map*.

In his three pages paper from 1875 [18], Lüroth proved that, whenever a curve can be parametrized by rational functions, one can find a rational parametrization that is one-to-one. In other words, the notions of uni-rationality and rationality are equivalent for the case of curves.

For many affine plane curves, we can find a parametrization through simple geometric arguments. As an example, let us construct a rational parametrization for the unit circle, which is defined by the equation $x^2 + y^2 - 1 = 0$. Consider a fixed point P on the circle and a variable point Q moving on a line not passing through P . Look at the second point of intersection R of the line PQ with the circle. Notice that, if Q traces its line, then R traces the circle. If we fix $P = (-1, 0)$ and assume Q to move along the y -axis, i.e., $Q = (0, t)$, then the equation of the line PQ is given by $y = t(1 + x)$. Next, we determine the intersection points of the line $PQ : y = t(1 + x)$ and the circle $x^2 + y^2 = 1$ which leads us to the equation

$$t^2(1+x)^2 = y^2 = 1 - x^2 = (1-x)(1+x).$$

We see that the first point of intersection is $P = (-1, 0)$. For the coordinates of the point R , we find

$$\begin{aligned} t^2(1+x) &= (1-x) \\ t^2 + t^2x &= 1 - x \\ x &= \frac{1 - t^2}{1 + t^2} \end{aligned}$$

and $y = t(1+x) = 2t/(1+t^2)$. Finally, recall that R traces the circle for varying values of t . Therefore, the coordinates of R provide us with the sought-after rational parametrization:

$$R = (\phi_x(t), \phi_y(t)) = \left(\frac{1 - t^2}{1 + t^2}, \frac{2t}{1 + t^2} \right)$$

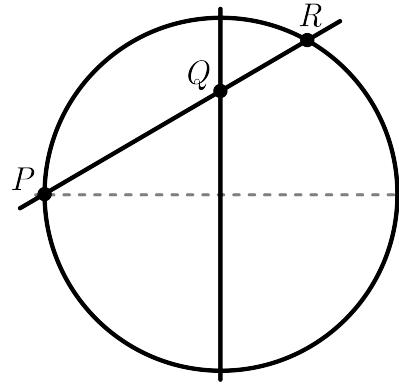


FIGURE 1.1. Parametrization of the unit circle by a family of lines.

While the first geometric parametrization of a curve appeared in the works of Newton [19], there is remarkable evidence that similar techniques were already known to the ancient Babylonians in 1500 BC [20] to systematically generate the famous Pythagorean triples, i.e., triples (a, b, c) of natural numbers that satisfy the equation $a^2 + b^2 = c^2$.

Furthermore, we should mention that one can use the above method to parametrize any affine plane curve that is defined by an irreducible degree-2 polynomial. This brings us to the fundamental question:

Which curves admit a rational parametrization?

The answer was found in 1865 by Clebsch [21], who proved that curves can be parametrized by rational functions if and only if a certain birational invariant, called the *genus*, is equal to 0.

To get an idea of how to compute this quantity, let us consider an affine plane curve C defined by a degree- d polynomial equation $f(x, y) = 0$. Through *homogenization* of f , we obtain a degree- d homogeneous polynomial

$$F(x, y, z) := z^d f(x/z, y/z),$$

which defines a *projective curve*

$$\overline{C} := \{[x : y : z] \in \mathbb{P}^2 \mid F(x, y, z) = 0\} \subset \mathbb{P}^2.$$

We call \overline{C} the *projective closure* of the affine curve C . Provided that \overline{C} is smooth, we can compute its genus as

$$g(\overline{C}) = \frac{(d-1)(d-2)}{2},$$

and define the genus of the affine curve C to be the genus of its projective closure.

In general, however, \overline{C} will not be smooth. We say that a point $p \in \overline{C}$ is a *singular point* of \overline{C} if

$$\frac{\partial}{\partial x} f(p) = \frac{\partial}{\partial y} f(p) = \frac{\partial}{\partial z} f(p) = 0,$$

and write Σ for the *singular locus*, i.e., the set of singular points of \overline{C} . The most common singularities are the *ordinary double point* and the *cusp*.

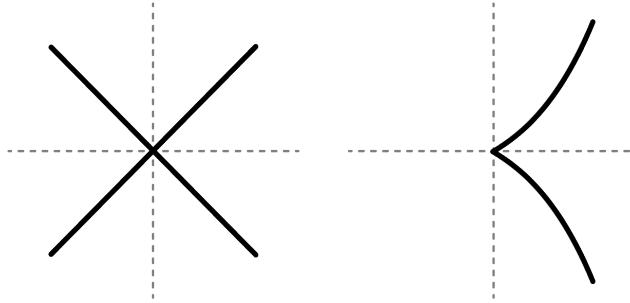


FIGURE 1.2. The ordinary double point and the cusp.

To each singular point $p \in \overline{C}$, we can associate an integer $\delta(\overline{C}, p)$, called the δ -*invariant* or *virtual number of double points*. Some important values are that of the cusp with $\delta = 1$ and that of the *ordinary m-point*, i.e., the intersection of m lines that have pairwise different tangents. The δ -invariant of such points is $\delta = m(m - 1)/2$. One can compute the genus of a curve through its degree and the δ -invariant of its singular points via

$$g(\overline{C}) = \frac{(d-1)(d-2)}{2} - \sum_{p \in \Sigma} \delta(\overline{C}, p).$$

Notice that, by the above formula and Clebsch's criterion, a degree- d curve whose singular locus is given by r ordinary double points is parametrizable by rational functions if and only if

$$r = \frac{(d-1)(d-2)}{2}.$$

In particular, an irreducible degree-3 curve with an ordinary double point is rational. Consider, for example, the nodal cubic C' defined by $y^2 - x^3 - x^2 = 0$.

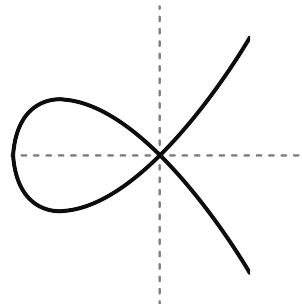


FIGURE 1.3. The nodal cubic.

The projective closure of C' has an ordinary double point, namely $p = [0 : 0 : 1]$. Therefore, we have $g(C') = 0$, telling us that C' is a rational curve. Furthermore, we will see in Part 3 that the existence of a double point allows us to parametrize any irreducible degree-3 curve similarly to the circle, namely by intersecting it with a family of lines through the double point.

It is, however, not always possible to find a parametrization in that way. A simple counterexample is the lemniscate—a degree-4 curve whose projective closure has 3 double points and, therefore, genus 0. Though rational, one cannot parametrize the lemniscate by a family of lines [22]. Nevertheless, one can use a more general method and parametrize through curves of higher degree. In fact, this more general method can be used to find a rational parametrization of any genus-0 curve [23].

To conclude this section, let us come back to the study of abelian integrals. Recall that we want to know under which circumstances we can reduce an abelian integral

$$\int R(x, y) \, dx$$

to a primitive of a univariate rational function. We now see that this is always the case if the curve that the abelian integral “depends” on is a rational curve.

For example, we can use the parametrization of the unit circle in the simple case where $R(x, y) = 1/y$ with $y = \sqrt{1 - x^2}$ to compute

$$\int \frac{dx}{\sqrt{1 - x^2}} = \int \frac{dx}{y} = -2 \int \frac{dt}{1 + t^2} = i \log \left(\frac{1 + iz}{1 - iz} \right) + c$$

with c being a complex constant.

More generally, if an abelian integral “depends” on a curve that is defined by $f(x, y) = 0$ and if $(\phi_x(t), \phi_y(t))$ is a rational parametrization for this curve, then we can reduce the abelian integral via

$$\int R(x, y) \, dx = \int R(\phi_x(t), \phi_y(t)) \phi'_x(t) \, dt,$$

where the right-hand side is indeed a primitive of a rational function.

In particular, since any curve defined by $y^2 = ax^2 + bx + c$, with complex coefficients a , b , and c , can be parametrized similarly to the circle, we can reduce any abelian integral

$$\int R(x, \sqrt{ax^2 + bx + c}) dx$$

to a primitive of a rational function. The corresponding variable changes are also known as *Euler substitutions*.

On the other hand, we see that abelian integrals involving smooth degree-3 curves like $y^2 = 1 - x^3$ cannot be reduced to primitives of a rational function since $y^2 = 1 - x^3$ defines a curve of genus 1. Rather, the abelian integral belongs, in general, to a new class of functions called *elliptic integrals*.

Let us, however, clarify a common misconception about the *elementarity* of abelian integrals. We say that a given function is *elementary* if it is a finite composition of logarithms, exponentials, and algebraic functions. In particular, the above mentioned class of elliptic integrals is *not* elementary. Clearly, abelian integrals that are reducible to a primitive of a rational function are elementary because we can write them as a sum of logarithms plus a rational function. There are, however, some special cases in which the abelian integral involves a *non-rational* curve but is still elementary. A trivial example is given by

$$\int \frac{3x^2 + 2x + 1}{\sqrt{x^3 + x^2 + x + 1}} dx = \log \left(\sqrt{x^3 + x^2 + x + 1} \right) + c$$

with c being a complex constant. A less obvious example is the integral

$$\int \frac{x}{\sqrt{x^4 + 10x^2 - 96x - 71}} dx,$$

which can be expressed in terms of elementary functions as well [24]. The corresponding expression is given by

$$\begin{aligned} & -\frac{1}{8} \log \left((x^6 + 15x^4 - 80x^3 + 27x^2 - 528x + 781) \sqrt{x^4 + 10x^2 - 96x - 71} \right. \\ & \left. - x^8 - 20x^6 + 128x^5 - 54x^4 + 1408x^3 - 3124x^2 - 10001 \right) + c, \end{aligned}$$

where c is, again, a complex constant.

The two difficult problems of

1. deciding under which circumstances a given integral is elementary, and
2. how to obtain a solution in terms of elementary functions

were finally solved by Liouville [25]–[27] and Risch [28], [29]. Special integrals like the above examples, i.e., integrals that are elementary although they “depend” on a non-rational curve are, however, the exception rather than the norm.

1.3. THE RATIONALITY QUESTION IN HIGHER DIMENSIONS

Now that we have discussed the rationality question for curves, let us give a brief overview of what is known beyond the one-dimensional case. Historically, after the extensive study of curves, the next logical step was to develop a birationally invariant theory of surfaces. While it was clear that any irreducible surface of degree two can be parametrized through a family of lines, the first interesting insights started with the study of smooth cubic surfaces, i.e., surfaces of degree three.

In 1849, Cayley observed that the number of straight lines on a smooth cubic surface must be finite, and Salmon found this number to be 27 [30], [31]. One decade later, Clebsch gave the explicit equation of a degree-9 surface that intersects the cubic surface exactly in its 27 lines [32], proving both the existence and the number of lines on smooth cubic surfaces. It was also Clebsch who first proved in 1866 that smooth cubic surfaces are always rational [33].

After those important contributions, Enriques and Castelnuovo finally succeeded in giving a rationality criterion for surfaces. They showed that a surface is rational if and only if its irregularity and its second plurigenus both vanish [34]. In particular, their results implied that uni-rationality and rationality are equivalent for surfaces.

Beyond two dimensions, however, things become considerably more complicated since uni-rationality and rationality are no longer equivalent, i.e., the existence of a rational parametrization does no longer imply the existence of a rational parametrization that is one-to-one. Even the case of threefolds is still not fully

understood, but there are some important results that we should mention:

- Any smooth cubic threefold is uni-rational but not rational [35].
- Any smooth quartic threefold is not rational [36]. There are, however, some quartic threefolds that are known to be uni-rational [37].
- Any smooth degree- d hypersurface in \mathbb{P}^n with $d \geq n + 1$ is not rational by a standard argument on the existence of holomorphic $(n - 1)$ -forms on such hypersurfaces.
- There is a particular double covering of \mathbb{P}^3 , branched along a quartic surface in \mathbb{P}^3 with ten nodes which is uni-rational but not rational [38].
- There are at least some cubic fourfolds that are known to be rational [39]. While most of them are expected to be irrational, there is not a single known example of a smooth cubic fourfold that is *proven* to be irrational.

Although we know very little about the rationality of hypersurfaces beyond two dimensions, we will see that the results for curves and surfaces already turn out to be very useful for various applications in contemporary high energy particle physics. However, before discussing these techniques in detail, let us first explain where the rationality question for algebraic hypersurfaces appears in physics computations.

CHAPTER 2

The Rationalization Question in High Energy Physics

2.1. FEYNMAN INTEGRALS

Theoretical predictions for collider experiments in high energy physics require the computation of Feynman integrals. Most Feynman integrals are difficult to compute and often divergent under the assumption of four-dimensional space-time. To deal with these divergences, physicists often calculate Feynman integrals via dimensional regularization, i.e., they replace the original integral in four dimensions with an integral in D dimensions [40]. This D is then assumed to depend on a small regularization parameter $\epsilon > 0$. In practice, one often assumes $D = 4 - 2\epsilon$ so that the physically relevant limit is recovered through $\epsilon \rightarrow 0$.

Every dimensionally regularized Feynman integral is a meromorphic function of the regularization parameter [41]–[43]. Thus, we can ask for the corresponding Laurent expansion. Because $\epsilon \rightarrow 0$ is the physical limit, we are particularly interested in the Laurent expansion around $\epsilon = 0$. For this reason, we may view a Feynman integral I as a Laurent series

$$I = \sum_{k \geq k_0} I_k \epsilon^k,$$

where $k_0 \in \mathbb{Z}$. The main objects of interest are, therefore, the coefficients I_k . So whenever we speak of computing a Feynman integral, we are referring to the computation of its Laurent coefficients. We will be particularly interested in the case when these coefficients have a representation in terms of MPLs.

2.2. DIFFERENTIAL EQUATIONS FOR FEYNMAN INTEGRALS

One of the predominant ways to compute Feynman integrals is the differential equations method [44]–[47]. To get an idea of how it works, let us sketch the calculation of two Feynman integrals that are relevant for the gauge boson self-energy in quantum electrodynamics (QED). The explicit integrals read

$$I_1 = (m^2)^{2-\frac{D}{2}} \int \frac{d^D k}{i\pi^{\frac{D}{2}}} \frac{1}{[m^2 - k^2]^2},$$

$$I_2 = (m^2)^{3-\frac{D}{2}} \int \frac{d^D k}{i\pi^{\frac{D}{2}}} \frac{1}{[m^2 - k^2]^2 [m^2 - (k - p)^2]}.$$

Working in dimensional regularization, we assume $D = 4 - 2\epsilon$. Furthermore, we may regard I_1 and I_2 as functions of $x = p^2/m^2$, where m is a particle mass and p is a particle momentum.

The two integrals I_1 and I_2 represent a particular choice of what is called a basis of master integrals. More precisely, all Feynman integrals that are relevant for the sought-after theoretical prediction can be reduced to I_1 and I_2 . The choice of a master integral basis is, however, not unique, and we will soon see that some choices are more appropriate than others.

As functions of $x = p^2/m^2$, the integrals I_1 and I_2 satisfy

$$\frac{d}{dx} \begin{pmatrix} I_1 \\ I_2 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \frac{\epsilon}{4x} - \frac{\epsilon}{4(x-4)} & -\frac{1}{2x} - \frac{1+2\epsilon}{2(x-4)} \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \end{pmatrix}.$$

To derive this differential equation, one can use several different programs, for example, `LiteRed` [48]. Note that all matrix entries are *rational* functions of x .

Recall that we have some freedom in choosing a basis of master integrals. Thus, we may switch to a different set of master integrals that satisfies a simpler differential equation. More precisely, we want to choose master integrals such that the ϵ -dependence of the matrix is only given by a constant prefactor [49], [50]. Let us, therefore, switch from I_1 and I_2 to

$$J_1 = 2\epsilon I_1, \quad J_2 = 2\epsilon \sqrt{-x(4-x)} I_2.$$

Finding an optimal basis of master integrals is a non-trivial problem. However, Dlapa, Henn, and Yan recently presented an algorithm to find such a basis, which is applicable as soon as one of the initial master integrals has a particular property, called uniform weight. For details on this technique, we refer the reader to their recent paper [51], which appeared only a few weeks before this thesis was published.

The new choice of master integrals fulfills the following differential equation:

$$\frac{d}{dx} \vec{J} = \epsilon \begin{pmatrix} 0 & 0 \\ -\frac{1}{\sqrt{-x(4-x)}} & -\frac{1}{x-4} \end{pmatrix} \vec{J}.$$

Notice that the simplified ϵ -dependence comes with a penalty: one of the matrix entries is no longer a rational function but “depends” on a square root.

Recall that, viewing J_1 and J_2 as Laurent series in ϵ , our ultimate goal is to find analytic expressions for their Laurent coefficients. More precisely, we want to express them in terms of MPLs. What is hindering us, is the presence of the square root $\sqrt{-x(4-x)}$.

To solve this problem, we substitute

$$x = -\frac{(1-t)^2}{t}.$$

This turns all matrix entries into rational functions in t :

$$\frac{d}{dt} \vec{J} = \epsilon \begin{pmatrix} 0 & 0 \\ -\frac{1}{t} & \frac{1}{t} - \frac{2}{t+1} \end{pmatrix} \vec{J}.$$

With the simplified ϵ -dependence and rational matrix entries, it is now a standard exercise to solve the differential equation order by order in terms of MPLs.

2.3. THE RATIONALIZATION QUESTION FOR FEYNMAN INTEGRALS

The previous section provided a typical sample calculation of Feynman integrals. We have seen that one of the most demanding tasks in these computations is to find a substitution that transforms a given set of square roots into rational functions. In the above example, we only had to rationalize *one* square root in

one variable. In general, however, one has to rationalize a whole set of square roots that depend on several variables. This rationalization problem often marks an insurmountable difficulty for many practitioners.

The goal of this thesis is to tackle this problem systematically. The main questions we will ask are:

1. Can we establish systematic methods to rationalize a given set of square roots?
2. In case we are unable to rationalize: Can we find a rigorous proof that the given set of square roots is not rationalizable?

We will start out with a discussion of the second question in Part 2 and subsequently present systematic rationalization techniques as well as their implementation in the `RationalizeRoots` package [1]. Our methods will make extensive use of the fact that the rationalization problem for square roots is directly related to the rationality question for algebraic hypersurfaces.

For instance, we may associate a one-dimensional hypersurface to the square root $\sqrt{-x(4-x)}$, namely the plane affine curve C defined by $y^2 + x(4-x) = 0$. We can then use the rational parametrization

$$(\phi_x(t), \phi_y(t)) = \left(-\frac{(1-t)^2}{t}, \frac{1-t^2}{t} \right)$$

of C to rationalize $\sqrt{-x(4-x)}$. Indeed, $\phi_x(t)$ is precisely the substitution we used in the sample calculation of the previous section, while $\phi_y(t)$ gives us the rationalized version of the square root up to sign. Conversely, if C would not be a rational curve, then this would prove that one cannot find a rational substitution to rationalize the square root.

CHAPTER 3

Algebraic Hypersurfaces

Now that we have discussed the physical context of the rationalization problem, let us introduce the mathematical vocabulary that we will use throughout the thesis. Unless otherwise stated, we will always work over the field of complex numbers \mathbb{C} .

3.1. AFFINE HYPERSURFACES

An *affine hypersurface* V is the zero set $\mathbb{V}(f)$ of a non-constant polynomial $f \in \mathbb{C}[x_1, \dots, x_n]$ in n variables, embedded in \mathbb{C}^n :

$$V = \mathbb{V}(f) \subset \mathbb{C}^n.$$

We call f the *defining polynomial* of V . The *degree* of V is defined as the degree of f . Notice that the embedding is an essential part of the definition: without specifying the ambient space, the one-point set $\{0\} \subset \mathbb{C}$ could be confused with the y -axis in \mathbb{C}^2 since both are defined as the zeros of $f = x$. We will, therefore, agree on the convention to view the zero set of a polynomial in n variables as a subset of \mathbb{C}^n . Whenever there is an exception to this convention, the embedding will be specified.

Examples If $V = \mathbb{V}(f)$ is defined by a degree- d polynomial $f \in \mathbb{C}[x, y]$ in two variables, then V defines an *affine plane curve* of degree d . Curves of degree 1 are called *lines*, of degree 2 *conics*, of degree 3 *cubics*. The unit circle $\mathbb{V}(x^2 + y^2 - 1)$ is an example of a conic.

The zero set of a degree-1 polynomial is called an *affine hyperplane*. For instance, the line $\mathbb{V}(ax + by - c)$ with non-zero scalars a , b , and c , is an affine hyperplane in \mathbb{C}^2 . \diamond

If $f = \prod_{i=1}^m f_i^{k_i}$ is the defining polynomial of an affine hypersurface V , where f_i denote the irreducible factors of f and $m, k_1, \dots, k_m \in \mathbb{N}$, then $V_i = \mathbb{V}(f_i)$ is called a *component* of V . Every hypersurface V is the union of its components, i.e., $V = \bigcup_{i=1}^m V_i$. An affine hypersurface is said to be *irreducible* if it has only one component.

The defining polynomial is only unique up to multiplication by non-zero constants and powers of its irreducible factors. Affine hypersurfaces should, therefore, be defined via *reduced* polynomials, i.e., instead of taking the defining polynomial to be $\prod_{i=1}^m f_i^{k_i}$, we take $\prod_{i=1}^m f_i$. Notice that reduced polynomials must not be confused with irreducible polynomials. For example, the polynomial $f = x^2 - y^2 = (x + y) \cdot (x - y)$ is reduced but not irreducible.

Finally, a *rational parametrization* of an affine hypersurface $V = \mathbb{V}(f) \subset \mathbb{C}^n$ with $f \in \mathbb{C}[x_1, \dots, x_n]$ is an n -tuple of rational functions $(\phi_{x_1}(\underline{t}), \dots, \phi_{x_n}(\underline{t}))$ which depend on $n-1$ variables $\underline{t} = (t_1, \dots, t_{n-1})$ and define a dominant rational map $\phi : \mathbb{C}^{n-1} \rightarrow V$. This means that

1. for almost all parameter values $\underline{t} \in \mathbb{C}^{n-1}$, the n -tuple $(\phi_{x_1}(\underline{t}), \dots, \phi_{x_n}(\underline{t}))$ defines a point on V , provided that we exclude the parameter values for which the denominators of the ϕ_{x_i} vanish.
2. up to subsets $U \subset V$ of positive codimension, i.e., subsets of “measure zero,” we can write every point of V as an n -tuple $(\phi_{x_1}(\underline{t}), \dots, \phi_{x_n}(\underline{t}))$ for some \underline{t} of the parameter space \mathbb{C}^{n-1} .

3.2. PROJECTIVE SPACE

The *projective n -space* \mathbb{P}^n is the set of all complex lines through the origin in \mathbb{C}^{n+1} . If \sim denotes the equivalence relation of points lying on the same line through the origin, then

$$\mathbb{P}^n = \frac{\mathbb{C}^{n+1} \setminus \{0\}}{\sim}.$$

Points in \mathbb{P}^n are equivalence classes $[(x_0, \dots, x_n)] = \{(\lambda x_0, \dots, \lambda x_n)\}$, where λ can be any non-zero complex number and at least one of the coordinates x_i is non-zero. We denote an element $p \in \mathbb{P}^n$ by one of its representatives.

To distinguish the class from its representative, we use square brackets rather than parenthesis and write colons between the coordinates of the representing point:

$$[x_0 : \dots : x_n] \in \mathbb{P}^n.$$

These *homogeneous coordinates* emphasize that a point in \mathbb{P}^n is only defined up to a non-zero scalar multiple.

3.3. POINTS AT INFINITY

The projective space \mathbb{P}^n is often viewed as the complex n -space \mathbb{C}^n together with an “infinitely distant point in every direction.” To clarify this interpretation, consider the one-dimensional projective space \mathbb{P}^1 . If we fix a reference hyperplane in \mathbb{C}^2 , i.e., a complex line not passing through the origin, we obtain a representative for each point $p \in \mathbb{P}^1$ by taking the unique point where the reference line meets the line through the origin that defines p . Only one point in \mathbb{P}^1 fails to have such a representative, namely the point corresponding to the line through the origin that is parallel to the reference line. This point is called the *point at infinity*. Therefore, we can regard \mathbb{P}^1 as the union $\mathbb{C} \cup \{\infty\}$ via

$$[x_0 : x_1] \mapsto \begin{cases} \frac{x_1}{x_0}, & \text{for } x_0 \neq 0, \\ \infty, & \text{for } x_0 = 0. \end{cases}$$

To take this construction one step further, consider the projective plane \mathbb{P}^2 . First, we fix a reference hyperplane in \mathbb{C}^3 , i.e., a complex plane not passing through the origin. Almost all points in \mathbb{P}^2 will have a unique representative on this reference plane. The exceptions are the points corresponding to the

lines through the origin that are parallel to the reference plane. These *points at infinity* form a copy of \mathbb{P}^1 so that $\mathbb{P}^2 = \mathbb{C}^2 \cup \mathbb{P}^1$.

We can generalize this idea to the case of \mathbb{P}^n as follows: if U_{x_0} is the subset of \mathbb{P}^n in which the x_0 -coordinate is non-zero, then we can identify U_{x_0} with the hyperplane $x_0 = 1$ in \mathbb{C}^{n+1} via

$$[x_0 : x_1 : \dots : x_n] = \left[1 : \frac{x_1}{x_0} : \dots : \frac{x_n}{x_0} \right] \mapsto \left(1, \frac{x_1}{x_0}, \dots, \frac{x_n}{x_0} \right).$$

Thus, U_{x_0} is a copy of \mathbb{C}^n , and we may think of it as the “finite part” of \mathbb{P}^n . We will call the affine space that corresponds to U_{x_0} the *coordinate chart in which $x_0 = 1$* . The remaining points, for which $x_0 = 0$, are called the *points at infinity*. These are representatives of the lines through the origin in \mathbb{C}^{n+1} that are parallel to the reference hyperplane $x_0 = 1$. They form an $n - 1$ -dimensional projective space \mathbb{P}^{n-1} so that $\mathbb{P}^n = \mathbb{C}^n \cup \mathbb{P}^{n-1}$ via

$$[x_0 : \dots : x_n] \mapsto \begin{cases} \left(\frac{x_1}{x_0}, \dots, \frac{x_n}{x_0} \right), & \text{for } x_0 \neq 0, \\ [x_1 : \dots : x_n], & \text{for } x_0 = 0. \end{cases}$$

Notice that our choice of a reference hyperplane is arbitrary. For instance, instead of U_{x_0} , we could have considered any U_{x_i} with $0 \leq i \leq n$. Therefore, what is “finite” and what is “at infinity” is a matter of perspective—it depends on the coordinate chart that we are working in.

3.4. PROJECTIVE HYPERSURFACES

A polynomial $F \in \mathbb{C}[x_0, \dots, x_n]$ is called *homogeneous of degree d* if all its terms have the same degree d . In particular, a degree- d homogeneous polynomial satisfies

$$F(\lambda x_0, \dots, \lambda x_n) = \lambda^d F(x_0, \dots, x_n), \quad \lambda \in \mathbb{C}.$$

Notice that, if a point $(x_0, \dots, x_n) \in \mathbb{C}^{n+1}$ is a zero of a homogeneous polynomial F , then every point $(\lambda x_0, \dots, \lambda x_n)$ is a zero of F . Thus, the zero set of F is a union of complex lines through the origin in \mathbb{C}^{n+1} .

We define a *projective hypersurface* as the zero set of a homogeneous polynomial $F \in \mathbb{C}[x_0, \dots, x_n]$, embedded in \mathbb{P}^n :

$$V = \mathbb{V}(F) \subset \mathbb{P}^n.$$

Recall that U_{x_i} denotes the subset of \mathbb{P}^n in which the coordinate x_i is non-zero, and that U_{x_i} corresponds to a copy of \mathbb{C}^n , namely the coordinate chart of \mathbb{P}^n in which $x_i = 1$. Similarly, the intersection $V_{x_i} = V \cap U_{x_i} \subset \mathbb{P}^n$ corresponds to an affine hypersurface

$$\mathbb{V}(F(x_0, \dots, x_{i-1}, 1, x_{i+1}, \dots, x_n)) \subset \mathbb{C}^n,$$

called the *affine chart of V in which $x_i = 1$* . Notice that we can always regard a projective hypersurface as the union $V = \bigcup_{i=0}^{n+1} V_{x_i}$.

By abuse of notation, we will denote by U_{x_i} not only the subset of \mathbb{P}^n in which the coordinate x_i is non-zero, but also the coordinate chart of \mathbb{P}^n in which $x_i = 1$. Likewise, we will denote by V_{x_i} not only the intersection $V \cap U_{x_i} \subset \mathbb{P}^n$, but also the affine chart of V in which $x_i = 1$.

Example The affine charts of $W = \mathbb{V}(x^2 + y^2 - z^2) \subset \mathbb{P}^2$ are given by the hyperbolas $W_x = \mathbb{V}(1 + y^2 - z^2) \subset \mathbb{C}^2$ and $W_y = \mathbb{V}(x^2 + 1 - z^2) \subset \mathbb{C}^2$ together with the complex unit circle $W_z = \mathbb{V}(x^2 + y^2 - 1) \subset \mathbb{C}^2$. Notice that we can find a representative for each point of W in at least one of its affine charts. Put differently, for every point $p \in W$, we can always find at least one affine chart of W so that p is not “at infinity.” \diamond

3.5. PROJECTIVE CLOSURE OF AN AFFINE HYPERSURFACE

The *projective closure* of an affine hypersurface $V = \mathbb{V}(f) \subset \mathbb{C}^n$ is the projective hypersurface $\overline{V} = \mathbb{V}(F) \subset \mathbb{P}^n$, defined by the *homogenization* F of f . We can *homogenize* a degree- d polynomial f in n variables to turn it into a degree- d homogeneous polynomial F in $n+1$ variables in the following way: decompose f into the sum of its *homogeneous components* of various degrees, i.e., write $f = g_0 + \dots + g_d$, where the g_i are homogeneous polynomials of degree i . Notice that some g_i ’s may be zero, but $g_d \neq 0$. The homogeneous component g_d is

already homogeneous of degree d . The term $g_{d-1} \in \mathbb{C}[x_1, \dots, x_n]$, however, is homogeneous of degree $d-1$. To make it homogeneous of degree d as well, we multiply by a new variable x_0 and obtain a polynomial $x_0 g_{d-1} \in \mathbb{C}[x_0, \dots, x_n]$. In the same manner, we turn all of the remaining g_i 's into a homogeneous degree- d polynomials via multiplication by x_0^{d-i} . The sum of these terms is the homogenization of f , a degree- d homogeneous polynomial

$$F = x_0^d g_0 + x_0^{d-1} g_1 + \dots + g_d.$$

We call x_0 the *homogenizing variable*. Notice that the restriction of F to the hyperplane $x_0 = 1$ recovers the original polynomial f .

Example The projective closure \bar{V} of the unit circle $V = \mathbb{V}(x^2 + y^2 - 1) \subset \mathbb{C}^2$ is given by the projective hypersurface $\bar{V} = \mathbb{V}(x^2 + y^2 - z^2) \subset \mathbb{P}^2$. We see that the unit circle has two points “at infinity.” Put differently, we see that \bar{V} has two points that lack a representative in the affine chart V of \bar{V} in which $z = 1$. These two points are given by $[1 : i : 0]$ and $[1 : -i : 0]$. \diamond

3.6. SINGULAR POINTS OF HIGH MULTIPLICITY

The *tangent space* $T_p V$ at a point $p = (p_1, \dots, p_n) \in V$ of an affine hypersurface $V = \mathbb{V}(f) \subset \mathbb{C}^n$ with defining polynomial $f \in \mathbb{C}[x_1, \dots, x_n]$ is the affine hyperplane with defining polynomial

$$\sum_{i=1}^n \frac{\partial f}{\partial x_i}(p) \cdot (x_i - p_i).$$

A point $p \in \mathbb{C}^n$ is a *singular point* of V if it does not allow for a well-defined tangent space, i.e., if

$$f(p) = \frac{\partial f}{\partial x_1}(p) = \dots = \frac{\partial f}{\partial x_n}(p) = 0.$$

We say that $p \in V$ is a *regular point* of V , if it is not a singular point of V .

A point $p \in V$ is of *multiplicity* $r \in \mathbb{N}$ if there exists at least one non-vanishing r -th partial derivative

$$\frac{\partial^{i_1+\dots+i_n} f}{\partial x_1^{i_1} \dots \partial x_n^{i_n}}(p) \neq 0 \text{ with } i_1 + \dots + i_n = r$$

and, at the same time, all lower-order partial derivatives vanish at p :

$$\frac{\partial^{i_1+\dots+i_n} f}{\partial x_1^{i_1} \dots \partial x_n^{i_n}}(p) = 0 \text{ with } i_1 + \dots + i_n = k \text{ for all } k = 0, \dots, r-1.$$

We write $\text{mult}_p(V) = r$. Notice that the regular points of V are precisely the points of multiplicity 1. Later, in Part 3, we will be particularly interested in the points of V with multiplicity $d-1$, where d denotes the degree of V . We will often speak of these points as *$(d-1)$ -points*, implicitly assuming that d denotes the degree of the hypersurface under consideration.

The above notions carry over to the case of projective hypersurfaces in an obvious way: If $V = \mathbb{V}(F) \subset \mathbb{P}^n$ denotes a projective hypersurface defined by a homogeneous polynomial $F \in \mathbb{C}[x_0, \dots, x_n]$, then a singular point of V is a point where all $n+1$ partial derivatives of F vanish. A point $p \in V$ is of multiplicity r if there is at least one non-vanishing r -th partial derivative of F at p and, at the same time, all lower-order partial derivatives of F vanish at p .

Example The nodal cubic has defining polynomial $f(x, y) = y^2 - x^3 - x^2$, and a singular point at $p = (0, 0)$ since $f(p) = \frac{\partial f}{\partial x}(p) = \frac{\partial f}{\partial y}(p) = 0$. Furthermore, we see that $\frac{\partial^2 f}{\partial y^2}(p) \neq 0$, telling us that the nodal cubic has a point of multiplicity 2 at the origin. \diamond

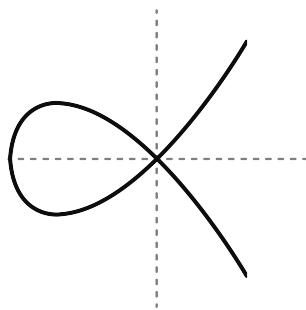


FIGURE 3.1. The nodal cubic $\mathbb{V}(y^2 - x^3 - x^2)$.

Notice that if we assume a given affine hypersurface to contain the origin, then we can define the multiplicity of the origin as the minimum degree of the non-zero homogeneous components of the defining polynomial. Since the notion of multiplicity is invariant under linear changes of coordinates, we can also determine the multiplicity of *any* point of the hypersurface by moving the point to the origin via a linear coordinate change and subsequently reading off the minimum of the degrees of the non-zero homogeneous components of the defining polynomial of the translated hypersurface.

So whenever we have a degree- d hypersurface $V = \mathbb{V}(f) \subset \mathbb{C}^n$ with a point $p = (p_1, \dots, p_n)$ of multiplicity $r < d$ and move $p = (p_1, \dots, p_n)$ to the origin by considering the hypersurface with defining polynomial

$$g(x_1, \dots, x_n) := f(x_1 + p_1, \dots, x_n + p_n),$$

then g can always be written as

$$g(x_1, \dots, x_n) = g_r(x_1, \dots, x_n) + \dots + g_d(x_1, \dots, x_n),$$

where g_k denote degree- k homogeneous components of g with $k = r, \dots, d$.

3.7. SIMPLE SINGULARITIES OF CURVES

To conclude the present chapter, let us sketch some ideas behind the theory of plane curve singularities. On the one hand, this subject requires many notions that most physicists will not be familiar with. On the other hand, we will be able to perform the relevant techniques in an automated fashion using the `ClassSing` function [52]. It is, therefore, much more in line with the idea of this thesis to acquaint the reader with some *intuition* behind plane curve singularities, rather than to elaborate the theory in detail. We do, however, strongly recommend the book by Greuel, Lossen, and Shustin [53] for a thorough treatment of the subject.

In Chapter 1, we have already seen two different *types* of plane curve singularities, namely the cusp and the ordinary double point. This raises the question, whether one can develop a reasonable *classification* of singularities.

As an example, consider the affine plane curves $\mathbb{V}(y^2 - x^2)$ and $\mathbb{V}(y^2 - x^3 - x^2)$, whose real points are depicted below.

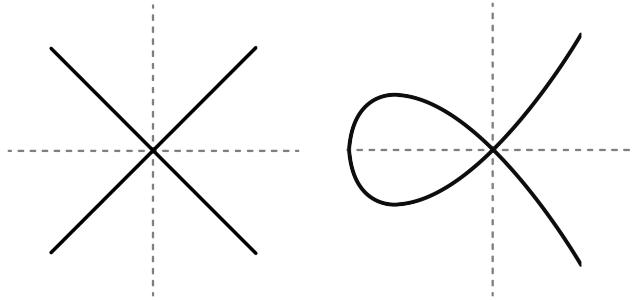


FIGURE 3.2. The curves $\mathbb{V}(y^2 - x^2)$ and $\mathbb{V}(y^2 - x^3 - x^2)$.

Both curves have a singular point at the origin. From a geometric point of view, it is evident that, taking successively smaller neighborhoods around the origin, the two curves look increasingly similar. Thus, in an attempt to classify plane curve singularities, it would be reasonable to require that these two singularities should belong to the same class.

We can encode such similarities algebraically by regarding defining polynomials of curves as elements of the *ring of formal power series* $\mathbb{C}[[x, y]]$. More precisely, if $C_1 = \mathbb{V}(f_1)$ and $C_2 = \mathbb{V}(f_2)$ denote two affine plane curves that both have a singularity at the origin, then we say that these two singularities are *of the same type* if the two quotient rings $\mathbb{C}[[x, y]]/\langle f_1 \rangle$ and $\mathbb{C}[[x, y]]/\langle f_2 \rangle$ are isomorphic. We call $\mathbb{C}[[x, y]]/\langle f_i \rangle$ the *associated quotient ring* of C_i .

Example For the two curves $\mathbb{V}(y^2 - x^2)$ and $\mathbb{V}(y^2 - x^3 - x^2)$, we can find an isomorphism between the associated quotient rings as follows: first, notice that the polynomial $f_2 = y^2 - x^3 - x^2$ is, in contrast to $f_1 = y^2 - x^2$, an irreducible element of $\mathbb{C}[x, y]$. If we, however, regard f_2 as an element of $\mathbb{C}[[x, y]]$, then we can write

$$f_2 = \left(y - x - \sum_{n=1}^{\infty} \frac{(-1) \cdots (1 - 2n)}{2^n} x^{n+1} \right) \times \\ \left(y + x + \sum_{n=1}^{\infty} \frac{(-1) \cdots (1 - 2n)}{2^n} x^{n+1} \right).$$

This factorization is easily obtained by observing that

$$f_2 = y^2 - x^2(1+x) = (y - x\sqrt{1+x})(y + x\sqrt{1+x})$$

and expanding

$$\sqrt{1+x} = 1 + \sum_{n=1}^{\infty} \frac{(-1) \cdots (1-2n)}{2^n} x^n.$$

Finally, the sought-after isomorphism between the rings $\mathbb{C}[[x, y]]/\langle y^2 - x^2 \rangle$ and $\mathbb{C}[[x, y]]/\langle y^2 - x^3 - x^2 \rangle$ is given by the map

$$(x, y) \mapsto \left(x + \sum_{n=1}^{\infty} \frac{(-1) \cdots (1-2n)}{2^n} x^{n+1}, y \right),$$

showing that C_1 and C_2 have a singularity of the same type at the origin. \diamond

In the late 1960's, Arnold started the classification of hypersurface singularities. Those efforts culminated in the famous list of *ADE singularities* [54], [55].

Definition If an affine hypersurface $V = \mathbb{V}(f) \subset \mathbb{C}^n$ has a singular point at the origin of \mathbb{C}^n , then we say that the origin is a *simple* or *ADE singularity* of V , if the associated quotient ring is isomorphic to a quotient ring $\mathbb{C}[[x_1, \dots, x_n]]/\langle g \rangle$, where g is a polynomial from the following list:

$$A_k : x_1^{k+1} + x_2^2 + q, \quad k \geq 1,$$

$$D_k : x_2(x_1^2 + x_2^{k-2}) + q, \quad k \geq 4,$$

$$E_6 : x_1^3 + x_2^4 + q,$$

$$E_7 : x_1(x_1^2 + x_2^3) + q,$$

$$E_8 : x_1^3 + x_2^5 + q,$$

where $q := x_3^2 + \cdots + x_n^2$. \diamond

The type of a singularity is invariant under linear coordinate transformations [53]. Therefore, we can classify any singular point $p = (p_1, \dots, p_n)$ of a given affine hypersurface $V = \mathbb{V}(f(x_1, \dots, x_n)) \subset \mathbb{C}^n$ by classifying the origin singularity of $V' = \mathbb{V}(f(x_1 + p_1, \dots, x_n + p_n)) \subset \mathbb{C}^n$. Further, if F denotes a

homogeneous polynomial in $n + 1$ variables, we say that a projective hypersurface $W = \mathbb{V}(F) \subset \mathbb{P}^n$ has a simple singularity at $q \in W$, if there is an affine chart of W , in which q is not “at infinity,” that has a simple singularity at the respective affine representative of q . The type of the singularity does not depend on the choice of the affine chart [53].

Note that many common hypersurface singularities, like the ordinary double point or the cusp, are simple singularities. In particular, we see that the two curves of our example have an A_1 singularity at the origin since

$$\mathbb{C}[[x, y]]/\langle y^2 - x^3 - x^2 \rangle \simeq \mathbb{C}[[x, y]]/\langle y^2 - x^2 \rangle \simeq \mathbb{C}[[x, y]]/\langle x^2 + y^2 \rangle.$$

To have some concrete examples in mind, the figures below depict the affine curve singularities of type A_1, \dots, A_4 and D_4, \dots, D_7 .

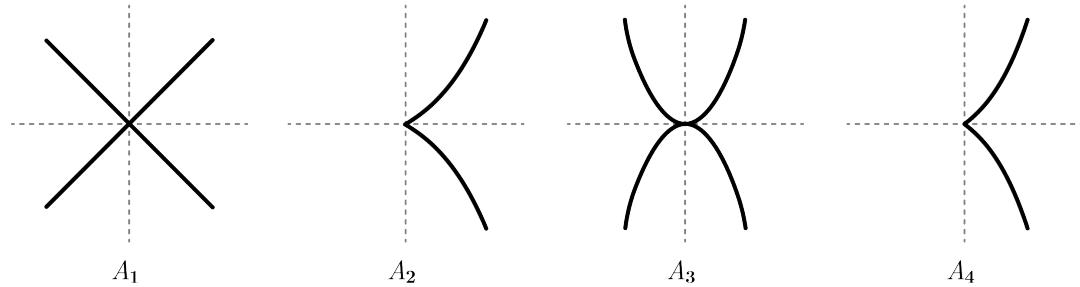


FIGURE 3.3. The first four A_k curve singularities.

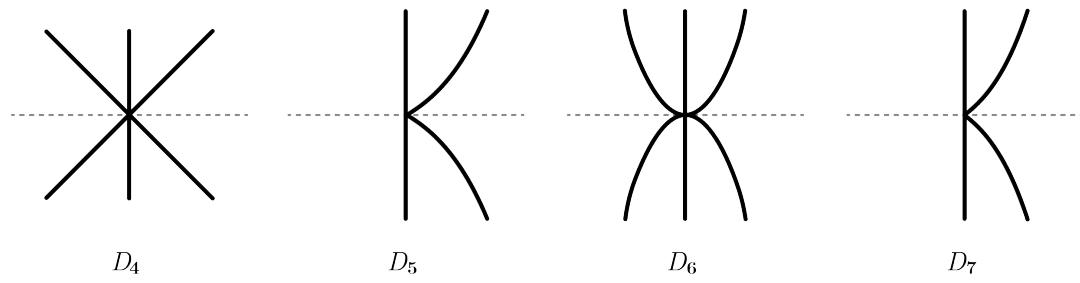


FIGURE 3.4. The first four D_k curve singularities.

These singularity types will play an important role in our non-rationalizability proofs for certain sets of square roots from high energy physics.

Theoretical physicists will, of course, be particularly interested in *how* to classify hypersurface singularities. What is needed is a simple, preferably automated, way to solve the classification problem for physically relevant examples. While some cases allow for a full classification by plain geometric reasoning, we will also present the `ClassSing` function, which one can use to automatically show that all singularities of a given curve are simple.

Part 2

Non-Rationalizable Square Roots

CHAPTER 4

Rationalizability

While many physically relevant sets of square roots are rationalizable, there are also various cases where a rationalization is not possible. Therefore, let us start with a discussion on how to prove such non-rationalizability statements before proceeding to the rationalization techniques of Part 3.

4.1. THE NOTION OF RATIONALIZABILITY

A square root \sqrt{p} with $p \in \mathbb{C}[x_1, \dots, x_n]$ is called *rationalizable* if and only if the affine hypersurface $V = \mathbb{V}(f) \subset \mathbb{C}^{n+1}$ with $f(r, x_1, \dots, x_n) = r^2 - p(x_1, \dots, x_n)$ has a rational parametrization.

Example The square root $\sqrt{-x(4-x)}$ is rationalizable. A rational parametrization of $V = \mathbb{V}(r^2 + x(4-x))$ has been given in Chapter 2. \diamond

More generally, if $p_1, \dots, p_m \in \mathbb{C}[x_1, \dots, x_n]$ are polynomials, then the set of square roots

$$\{\sqrt{p_1}, \dots, \sqrt{p_m}\}$$

is called *rationalizable* if and only if there are n rational functions $\phi_{x_1}, \dots, \phi_{x_n} \in \mathbb{C}(t_1, \dots, t_n)$ and m rational functions $\phi_{r_1}, \dots, \phi_{r_m} \in \mathbb{C}(t_1, \dots, t_n)$ such that, for all $k = 1, \dots, m$, the $(n+1)$ -tuple $(\phi_{r_k}, \phi_{x_1}, \dots, \phi_{x_n})$ is a rational parametrization for the hypersurface $\mathbb{V}(r_k^2 - p_k(x_1, \dots, x_n)) \subset \mathbb{C}^{n+1}$.

This is the same as saying that there is a single variable change in the x_i that rationalizes all of the given square roots simultaneously. If a parametrization of this form does not exist, we say that the set of square root is *not rationalizable* or call it a *non-rationalizable* set of square roots.

Example The set

$$\left\{ \sqrt{-x(4-x)}, \sqrt{x} \right\}$$

is rationalizable because there exist rational parametrizations

$$\begin{aligned} (\phi_{r_1}(t), \phi_x(t)) &= \left(\frac{(1-t^2)^2}{t^2}, \frac{(1-t)^4}{t^2} \right), \\ (\phi_{r_2}(t), \phi_x(t)) &= \left(\frac{(1-t)^2}{t}, \frac{(1-t)^4}{t^2} \right), \end{aligned}$$

for the two hypersurfaces $V_1 = \mathbb{V}(r_1^2 + x(4-x))$ and $V_2 = \mathbb{V}(r_2^2 - x)$ that share the same expression for ϕ_x . Put differently, there is a single rational substitution

$$x = \frac{(1-t)^4}{t^2}$$

that rationalizes all of the given square roots.

Conversely, the set

$$\left\{ \sqrt{-x(4-x)}, \sqrt{x+4} \right\}$$

is a non-rationalizable set of square roots. While we will discuss the techniques to prove such a statement in one of the upcoming chapters, the purpose of this example is rather to clarify the condition on the ϕ_{x_i} : at first sight, it may seem strange to call this set non-rationalizable because both square roots of the set are rationalizable—the first via the substitution from Chapter 2 and the second via $x = t^2 - 4$. These substitutions are, however, *not the same* and will, therefore, not be useful in Feynman integral computations. Instead, for practical applications in physics, we need a *single* substitution that rationalizes *all* of the given square roots and, as already touched upon above, such a substitution does not exist for the given set. \diamond

Notice that the definitions of this section also make sense for square roots with rational arguments, i.e., we could assume $p_1, \dots, p_m \in \mathbb{C}(x_1, \dots, x_n)$ instead of $p_1, \dots, p_m \in \mathbb{C}[x_1, \dots, x_n]$. It is, however, enough to consider polynomial square root arguments as guaranteed by the following lemma.

Lemma The set of square roots

$$\mathcal{R} = \left\{ \sqrt{\frac{f_1}{g_1}}, \dots, \sqrt{\frac{f_m}{g_m}} \right\},$$

with $f_1, \dots, f_m, g_1, \dots, g_m \in \mathbb{C}[x_1, \dots, x_n]$, is rationalizable if and only if the set

$$\mathcal{R}' = \left\{ \sqrt{f_1 \cdot g_1}, \dots, \sqrt{f_m \cdot g_m} \right\}$$

is rationalizable.

Proof If \mathcal{R} is rationalizable, then there exist m rational parametrizations $(\phi_{r_k}, \phi_{x_1}, \dots, \phi_{x_n})$ with $k = 1, \dots, m$ for the hypersurfaces with defining equations

$$r_1^2 = \frac{f_1}{g_1}, \dots, r_m^2 = \frac{f_m}{g_m}.$$

Therefore, these also solve the equations

$$r_1^2 = \frac{f_1 g_1}{g_1^2}, \dots, r_m^2 = \frac{f_m g_m}{g_m^2}.$$

But this means that the functions

$$\begin{aligned} \varphi_{r_k} &:= \phi_{r_k} \cdot g_k(\phi_{x_1}, \dots, \phi_{x_n}) \\ \varphi_{x_1} &:= \phi_{x_1} \\ &\vdots \\ \varphi_{x_n} &:= \phi_{x_n} \end{aligned}$$

give us m rational parametrizations $(\varphi_{r_k}, \varphi_{x_1}, \dots, \varphi_{x_n})$ that parametrize the hypersurfaces defined by

$$r_1^2 = f_1 \cdot g_1, \dots, r_m^2 = f_m \cdot g_m.$$

The converse statement is proven in the same manner and skipped for the sake of brevity. \square

In addition to this simple mathematical argument, the author is not aware of a single example from theoretical high energy physics where the initial set of

square roots that appears in a calculation contains non-polynomial arguments. Therefore, we will focus on sets of square roots with *polynomial* arguments. Notice, however, that we will only make this assumption in the context of non-rationalizability proofs. In the context of the rationalization methods of Part 3, square roots with rational arguments will be unavoidable and sometimes even be preferred over square roots with non-rational arguments.

4.2. ON THE SCOPE OF NON-RATIONALIZABILITY PROOFS

Most physicists have an intuitive idea of what the term “rationalizable square root” should imply, namely one’s ability to find a substitution that turns the given square root into a rational function. Most of the current physics literature does, however, not specify what *kind* of substitutions are allowed or excluded. It is tempting to discount this as an unnecessary detail, but it turns out that the situation is more delicate than one might think.

Consider, for example, the square root $\sqrt{t^4 + t^2 + 1}$. We will soon see that it corresponds to a non-rational plane affine curve and is, therefore, not rationalizable in the sense of the previous section. Nevertheless, we *can* find a substitution that rationalizes this square root, namely

$$t = \sqrt{\frac{(2-s) \cdot s}{s^2 - 1}},$$

which turns the square root under consideration into a rational function

$$\sqrt{t^4 + t^2 + 1} = \frac{s^2 - 1}{1 + s \cdot (s - 1)}.$$

As we see from this simple example, it is crucial to understand that our notion of non-rationalizability only implies that there is no *rational* substitution that rationalizes the given square root. It does, however, not exclude the existence algebraic substitutions as the one above. In the end, we are particularly interested in finding *rational* substitutions since they do not introduce new square roots in other parts of our computation. Algebraic substitutions, on the other hand, may rationalize the given square root, but will introduce new square roots in other places.

We should stress, though, that algebraic substitutions sometimes play an important role in intermediate steps when constructing a rational parametrization. In fact, we will present an example in Part 3 where it is necessary to use algebraic intermediate substitutions for our rationalization methods to succeed.

4.3. PROVING NON-RATIONALIZABILITY: THE STRATEGY

Our non-rationalizability proofs are always going to be proofs by contradiction and will rely on the following theorem:

Theorem If a given set of square roots

$$\{\sqrt{p_1}, \sqrt{p_2}, \dots, \sqrt{p_m}\}$$

with polynomial arguments $p_1, \dots, p_m \in \mathbb{C}[x_1, \dots, x_n]$ is rationalizable then, for every subset $\emptyset \neq J \subset \{1, \dots, m\}$, the hypersurface defined by the equation

$$r^2 = \prod_{j \in J} p_j$$

is parametrizable by rational functions.

Proof If the given set of square roots is rationalizable, then there exist m rational parametrizations of the form $(\phi_{r_k}, \phi_{x_1}, \dots, \phi_{x_n})$ with $k = 1, \dots, m$ that parametrize the m hypersurfaces defined by

$$r_1^2 = p_1, \dots, r_m^2 = p_m.$$

Using these parametrizations, we can construct a rational parametrization for every hypersurface of the form

$$r^2 = \prod_{j \in J} p_j$$

by mapping the rational functions that constitute the given parametrizations via

$$(\vec{r}, x_1, \dots, x_n) \mapsto \left(\prod_{j \in J} r_j, x_1, \dots, x_n \right),$$

where the entries of \vec{r} are formed by the variables r_j with $j \in J$. \square

Furthermore, we will make use of the following corollary.

Corollary If \mathcal{R} is a non-rationalizable set of square roots, then any larger set of square roots \mathcal{R}' that contains \mathcal{R} as a subset is also not rationalizable.

Proof Suppose \mathcal{R}' is a set of square roots that contains a non-rationalizable subset $\mathcal{R} = \{\sqrt{p_1}, \dots, \sqrt{p_m}\} \subset \mathcal{R}'$, where $1 \leq m \leq |\mathcal{R}'|$. If \mathcal{R}' would be rationalizable, then this would, in particular, imply the existence of a rational parametrization of the affine hypersurface defined by

$$r^2 = \prod_{j=1}^m p_j,$$

which contradicts the non-rationalizability of \mathcal{R} . \square

Based on these statements, we arrive at the following strategy to prove non-rationalizability of a given set of square roots \mathcal{R}' :

Strategy for Non-Rationalizability Proofs

1. Assume that a subset

$$\mathcal{R} = \{\sqrt{p_1}, \sqrt{p_2}, \dots, \sqrt{p_m}\} \subset \mathcal{R}'$$

of \mathcal{R}' is rationalizable.

2. By the above theorem, this implies that every hypersurface of the form

$$r^2 = \prod_{j \in J} p_j$$

has a rational parametrization. Therefore, consider any hypersurface of this form.

3. Prove that the hypersurface under consideration is not parametrizable by rational functions to contradict the assumption that \mathcal{R} is rationalizable.
4. Lastly, apply the above corollary to conclude that \mathcal{R}' is not rationalizable.

4.4. ON THE ROLE OF SQUARES

As explained in the previous section, we can prove the non-rationalizability of a given set of square roots

$$\{\sqrt{p_1}, \sqrt{p_2}, \dots, \sqrt{p_m}\}$$

by showing that at least one affine hypersurface of the form

$$r^2 = \prod_{j \in J} p_j$$

is not parametrizable by rational functions, where $p_1, \dots, p_m \in \mathbb{C}[x_1, \dots, x_n]$ and $\emptyset \neq J \subset \{1, \dots, m\}$.

Depending on the number of square roots m , one often has many different choices for a hypersurface of this type. While there may be many of these choices that will work to prove the non-rationalizability of the given set, some of the hypersurfaces will be more difficult to study than others. Therefore, one should try to pick the hypersurface that is easiest to investigate.

For instance, hypersurfaces of comparatively low degree will usually be easier to study than hypersurfaces of higher degree. Put differently, we usually want to pick the **minimum** number of polynomials p_j necessary for our hypersurface to be not parametrizable by rational functions.

Example Consider the set

$$\{\sqrt{(x-1)}, \sqrt{(x-2)(x-3)}, \sqrt{(x-4)(x-5)}\}.$$

Naively, we could take all square roots of the set into account and pick the affine plane curve $V = \mathbb{V}(r^2 - (x-1)(x-2)(x-3)(x-4)(x-5))$ as our hypersurface of choice. By the methods of the next chapter, one can then prove the non-rationalizability of the given set by showing that V is not parametrizable by rational functions.

On the other hand, we could also consider only the first two square root arguments and use $W = \mathbb{V}(r^2 - (x-1)(x-2)(x-3))$ instead of V , giving us an irrational curve as well, but being slightly easier to study. \diamond

In addition to the fact that we want to pick a hypersurface of a suitable degree, there is another—more subtle—condition that we want to impose on the defining equation of our hypersurface. For non-rationalizability proofs beyond square roots in one variable, our techniques will heavily rely on the presence of *simple* singularities. The singularities of the relevant hypersurface will, however, never be exclusively simple as soon as the right-hand side of the defining equation $r^2 = \prod_{j \in J} p_j$ contains a square.

For example, in the important case where the zeros of $\prod_{j \in J} p_j$ define a *one-dimensional* hypersurface, i.e., a curve, the presence of a square would imply that this affine plane curve has an entire *component* of higher multiplicity. In other words, the singular locus of this curve has dimension greater than zero, i.e., the set of singularities is not just a set of isolated points. Simple singular points are, however, necessarily *isolated*. Therefore, the presence of a single square on the right-hand side of $r^2 = \prod_{j \in J} p_j$ will immediately imply that not all singularities of the hypersurface are simple so that our main technique for square roots in two variables will not be applicable. Fortunately, the following lemma allows us to ignore all squares on the right-hand side of $r^2 = \prod_{j \in J} p_j$.

Lemma If $p, q \in \mathbb{C}[x_1, \dots, x_n]$ are non-constant polynomials, then the affine hypersurface $W = \mathbb{V}(r^2 - p \cdot q^2) \subset \mathbb{C}^{n+1}$ is parametrizable by rational functions if and only if $V = \mathbb{V}(r^2 - p) \subset \mathbb{C}^{n+1}$ is parametrizable by rational functions.

Proof If W is parametrizable by rational functions, then there exist rational functions $\phi_r, \phi_{x_1}, \dots, \phi_{x_n} \in \mathbb{C}(t_1, \dots, t_n)$ with

$$\phi_r^2 = p(\phi_{x_1}, \dots, \phi_{x_n}) \cdot (q(\phi_{x_1}, \dots, \phi_{x_n}))^2.$$

But this means that the functions $\phi_{x_1}, \dots, \phi_{x_n}$, and $\phi_{\tilde{r}} := \phi_r / (q(\phi_{x_1}, \dots, \phi_{x_n}))$ satisfy the equation $\tilde{r}^2 = p(x_1, \dots, x_n)$. The proof of the converse statement is just as simple and skipped for the sake of brevity. \square

Lastly, let us emphasize that “ignoring squares” means to ignore them entirely, e.g., we replace x^2 by 1 rather than by x .

4.5. When TO PROVE NON-RATIONALIZABILITY

When trying to prove the non-rationalizability of a given set of square roots, it is crucial to pick the right “starting point” for the proof. The problem is that certain substitutions can give the impression that rationalizable sets of square roots look like non-rationalizable ones. To clarify what we mean by this, let us discuss a simple example.

Example Consider the following set of square roots:

$$\{\sqrt{x-1}, \sqrt{x-2}\}.$$

In an attempt to rationalize this set, we may proceed as follows:

1. Try to rationalize the first square root.
2. If successful, plug the corresponding substitution into the second square root and try to rationalize the resulting square root.
3. If successful, compose both substitutions to obtain a single substitution that will rationalize both square roots.

In Part 3, we will discuss this procedure in more detail. For now, let us apply it to the example at hand: as a first step, we rationalize the first square root by putting $x = t^4 + 1$ so that

$$\sqrt{x-1} = t^2.$$

With this substitution, the second square root becomes

$$\sqrt{t^4 - 1},$$

giving us a square root of a degree-4 polynomial with distinct complex zeros. As we will see in the next chapter, this square root is not rationalizable. Therefore, it is very tempting to naively assume that the non-rationalizability of this square root implies non-rationalizability of the original set of square roots.

This assumption is, however, not true: suppose that we substitute $x = t^2 + 1$ instead of $x = t^4 + 1$ for the rationalization of the first square root. Clearly, the former is a valid substitution as well and yields

$$\sqrt{x - 1} = t$$

for the first square root and

$$\sqrt{x - 2} = \sqrt{t^2 - 1}$$

for the second. But the hypersurface corresponding to this new square root is just a plane conic curve so that we easily rationalize it with an Euler substitution. One of those is, for example, given by

$$t = \frac{2s^2}{1 - s^2} + 1.$$

Finally, the composition of these two substitutions yields a substitution that rationalizes both original square roots simultaneously and is given by

$$x = \left(\frac{2s^2}{1 - s^2} + 1 \right)^2 + 1,$$

showing that the given set of square roots is indeed rationalizable. \diamond

This example illustrates that proving non-rationalizability after some substitutions have already been made, does not necessarily imply non-rationalizability of the original set of square roots. For this reason, physicists should always prove non-rationalizability as early as possible, i.e., as soon as the square roots arise in the calculation. In typical physical applications like our sample calculation of Part 1, this means that one should always consider the square roots in the original kinematics in which they first appeared. In practice, these will often be given by squared masses and the common Mandelstam variables. The correct “starting point” to prove the non-rationalizability of a given set of square roots should, therefore, always be “as soon as they arise.”

CHAPTER 5

Sets of Square Roots in One Variable

In this chapter, we will explain how to prove non-rationalizability for sets of square roots in one variable. This means that we will only consider sets of the form

$$\{\sqrt{p_1}, \sqrt{p_2}, \dots, \sqrt{p_m}\},$$

where all square root arguments are polynomials $p_1, \dots, p_m \in \mathbb{C}[x]$ in a *single* variable x .

5.1. NON-RATIONALIZABILITY VIA GENUS

Recall from the previous chapter that, to show non-rationalizability of such a set, we have to find at least one hypersurface V of the form

$$r^2 = \prod_{j \in J} p_j$$

with $\emptyset \neq J \subset \{1, \dots, m\}$ such that V is not parametrizable by rational functions. In the case where all square root arguments are non-constant univariate polynomials depending on the same variable, this hypersurface V will always be a plane affine curve.

To prove the non-rationalizability of the given set, we need to show that V is not parametrizable by rational functions. As mentioned in Chapter 1, this problem was already solved by Clebsch [21] over 150 years ago. For our purposes, we may formulate Clebsch's result as follows:

Theorem A plane affine curve $V \subset \mathbb{C}^2$ is parametrizable by rational functions if and only if its genus is 0.

For a proof of this statement, we refer to the original work of Clebsch [21] or any textbook on basic algebraic geometry, e.g., the one by Shafarevich [56].

In Chapter 1, we have already seen how to compute the genus of a curve based on its degree and the δ -invariant of its singular points. The easiest and most reliable way to perform this computation is to use computer algebra software. In this thesis, we will use **Magma** [57] but there are many other programs, e.g., **Singular** [58] that will compute the genus just as fine.

Given the set

$$\{\sqrt{p_1}, \sqrt{p_2}, \dots, \sqrt{p_m}\},$$

the curves of interest are defined by polynomials of the form $f(r, x) = r^2 - p(x)$, where $p(x) = \prod_{j \in J} p_j$ with $\emptyset \neq J \subset \{1, \dots, m\}$.

In **Magma**, we can then compute the genus of one of these curves, call it V , with only a few lines of code

```
> A<r,x> := AffineSpace(Rationals(),2);
> f := r^2 - p(x);
> V := Curve(A,f);
> Genus(V);
```

where the polynomial $p(x) = \prod_{j \in J} p_j$ is to be substituted for the italic expression $p(x)$ in the definition of f . As soon as we find that such a curve has a non-zero genus, we can conclude that the given set is not rationalizable.

5.2. NON-RATIONALIZABILITY VIA DISTINCT ZEROS

Another straightforward way to prove the non-rationalizability of univariate sets of square roots is to check whether the polynomial $p(x) = \prod_{j \in J} p_j$, as defined in the previous section, has at least 3 distinct complex zeros of odd multiplicity. To see that this statement is indeed true, let us first consider the following lemma:

Lemma If $p \in \mathbb{C}[x]$ is a polynomial whose complex zeros are all distinct and $\deg(p) \geq 3$, then $V = \mathbb{V}(r^2 - p(x)) \subset \mathbb{C}^2$ is not parametrizable by rational functions.

Proof Using the definition of singular points, one can easily check that the affine curve $V = \mathbb{V}(r^2 - p(x))$ has a singular point if and only if $p(x)$ has a double zero. Thus, if all complex zeros of $p(x)$ are distinct, then V is smooth, and the statement follows from the genus formula

$$g = \frac{(d-1)(d-2)}{2}$$

for smooth degree- d curves together with Clebsch's genus criterion. \square

With the above lemma, we arrive at the following theorem:

Theorem If a degree- d polynomial $p \in \mathbb{C}[x]$ has at least 3 distinct complex zeros of odd multiplicity, then $V = \mathbb{V}(r^2 - p(x))$ is not parametrizable by rational functions.

Proof We write $n \leq d$ for the number of distinct zeros $a_i \in \mathbb{C}$ of p . Furthermore, we take $m := |\{a_i \in \mathbb{C} | p(a_i) = 0, \nu(a_i) \text{ is odd}\}|$ to be the number of zeros of p that have odd multiplicity, where $\nu(\cdot)$ denotes the multiplicity of a given zero of p . By assumption, we have $3 \leq m \leq n \leq d$. We write a_1, \dots, a_m for the zeros of odd multiplicity and a_{m+1}, \dots, a_n for the zeros of even multiplicity. Therefore, by the fundamental theorem of algebra, we have

$$\begin{aligned} p(x) &= \left(c \cdot \prod_{i=1}^m (x - a_i) \right) \cdot \left(\prod_{i=1}^m (x - a_i)^{\nu(a_i)-1} \right) \cdot \left(\prod_{i=m+1}^n (x - a_i)^{\nu(a_i)} \right) \\ &= \left(c \cdot \prod_{i=1}^m (x - a_i) \right) \cdot \left(\prod_{i=1}^m (x - a_i)^{\frac{\nu(a_i)-1}{2}} \right)^2 \cdot \left(\prod_{i=m+1}^n (x - a_i)^{\frac{\nu(a_i)}{2}} \right)^2, \end{aligned}$$

where $c \in \mathbb{C}$ is the leading coefficient of p . The lemma of Chapter 4 tells us that we can ignore squares in p , i.e., if $W = \mathbb{V}(r^2 - c \cdot \prod_{i=1}^m (x - a_i))$ is not parametrizable by rational functions, then $V = \mathbb{V}(r^2 - p(x))$ is not parametrizable by rational functions. But, by the previous lemma, it is clear that W is not parametrizable by rational functions. \square

In conclusion, to prove non-rationalizability of a univariate set of square roots

$$\{\sqrt{p_1}, \sqrt{p_2}, \dots, \sqrt{p_m}\},$$

one only needs to show that there is at least one polynomial $p(x) = \prod_{j \in J} p_j$ with $\emptyset \neq J \subset \{1, \dots, m\}$ that has at least 3 distinct complex zeros of odd multiplicity.

5.3. AN EXAMPLE FROM HIGH ENERGY PHYSICS

Sets of square roots in a single variable occurred in many Feynman integral computations, especially throughout the last decade [59]–[83]. Let us, therefore, show how the criteria of the previous sections are to be applied in practice. As an example, consider the set

$$\mathcal{R} = \left\{ \sqrt{x}, \sqrt{1+4x}, \sqrt{x(x-4)} \right\},$$

which appears in perturbative corrections for Higgs production [84]. Our goal is to show that these three square roots cannot be rationalized simultaneously. We prove this using the strategy of the previous chapter, i.e., we show that at least one hypersurface of the form $V = \mathbb{V}(r^2 - \prod_{j \in J} p_j)$ with $\emptyset \neq J \subset \{1, 2, 3\}$ and $p_1(x) = x, p_2(x) = 1+4x, p_3(x) = x(x-4)$ is not parametrizable by rational functions. For instance, consider the affine curve $V = \mathbb{V}(r^2 - p_2(x)p_3(x))$. On the one hand, we see that the polynomial $p_2(x)p_3(x)$ has 3 distinct complex zeros of multiplicity 1, namely $x_1 = -1/4, x_2 = 0$, and $x_3 = 4$. On the other hand, we can check that V has a non-zero genus with **Magma**:

```
> A<r,x> := AffineSpace(Rationals(), 2);
> f := r^2 - (1+4x)*x*(x-4);
> V := Curve(A,f);
> Genus(V);
1
```

We conclude that V cannot be parametrized by rational functions. Therefore, the square roots of \mathcal{R} cannot be rationalized simultaneously.

CHAPTER 6

Sets of Square Roots in Two Variables and Beyond

6.1. NON-RATIONALIZABILITY CRITERION

In this chapter, we will consider sets of square roots

$$\{\sqrt{p_1}, \sqrt{p_2}, \dots, \sqrt{p_m}\},$$

where all square root arguments are polynomials $p_1, \dots, p_m \in \mathbb{C}[x, y]$. To prove non-rationalizability of such a set, we have to find at least one hypersurface V of the form

$$r^2 = \prod_{j \in J} p_j$$

with $\emptyset \neq J \subseteq \{1, \dots, m\}$ such that V is not parametrizable by rational functions. We start our discussion with the following lemma.

Lemma If $F_{2k} \in \mathbb{C}[x, y, z]$ is the homogenization of a polynomial $f_{2k} \in \mathbb{C}[x, y]$ of even degree $2k$, where $k \geq 1$ and z denotes the homogenizing variable, then the hypersurface $V = \mathbb{V}(r^2 - f_{2k}(x, y)) \subset \mathbb{C}^3$ is parametrizable by rational functions if and only if $W = \mathbb{V}(r^2 - F_{2k}(x, y, z)) \subset \mathbb{C}^4$ is parametrizable by rational functions.

Proof If $(\phi_r(t_1, t_2), \phi_x(t_1, t_2), \phi_y(t_1, t_2))$ is a rational parametrization of V then, because the homogenization of $f_{2k}(x, y)$ is defined as

$$F_{2k}(x, y, z) := z^{2k} f_{2k}(x/z, y/z),$$

we can define

$$\begin{aligned}
\phi'_r(t_1, t_2, t_3) &:= t_3^k \phi_r(t_1, t_2), \\
\phi'_x(t_1, t_2, t_3) &:= t_3 \phi_x(t_1, t_2), \\
\phi'_y(t_1, t_2, t_3) &:= t_3 \phi_y(t_1, t_2), \\
\phi'_z(t_1, t_2, t_3) &:= t_3,
\end{aligned}$$

which gives us a rational parametrization $(\phi'_r, \phi'_x, \phi'_y, \phi'_z)$ of W since

$$\begin{aligned}
(\phi'_r)^2 &= t_3^{2k} \cdot \phi_r^2 \\
&= t_3^{2k} \cdot f_{2k}(\phi_x, \phi_y) \\
&= (\phi'_z)^{2k} \cdot f_{2k}(\phi'_x/\phi'_z, \phi'_y/\phi'_z) \\
&= F_{2k}(\phi'_x, \phi'_y, \phi'_z).
\end{aligned}$$

The proof of the converse direction is just as simple and skipped for the sake of brevity. \square

Let us now formulate the criterion that we will use for our non-rationalizability proofs in the two-variable case.

Theorem If $F_{2k} \in \mathbb{C}[x, y, z]$ is a homogeneous polynomial of degree $2k$ with $k \geq 3$, and if the projective curve $B = \mathbb{V}(F_{2k}(x, y, z)) \subset \mathbb{P}^2$ has only simple singularities, then $V = \mathbb{V}(r^2 - F_{2k}(x, y, z)) \subset \mathbb{C}^4$ is not parametrizable by rational functions.

Proof A detailed proof of this theorem requires notions whose introduction goes beyond the point of this thesis. We should, however, provide the key arguments for the reader that is familiar with those notions. Furthermore, we give a few short comments for physicists in the form of indented text blocks to spark some intuition behind the mathematical vocabulary. For a thorough treatment, we refer to Section 22 of Chapter 5 in [85], and to [86] for an introduction to the theory of weighted projective spaces.

We may view V as a two-dimensional hypersurface in the weighted projective space $\mathbb{P}(k, 1, 1, 1)$, where x , y , and z are homogeneous coordinates of weight 1, and r is a homogeneous coordinate of weight k .

Weighted projective spaces are a generalization of the projective spaces \mathbb{P}^n . They are obtained by changing the *weight* of the coordinates of the space and, hence, changing the condition for a polynomial to be homogeneous. For example, in a space in which the coordinates x_0 and x_1 have weight 1 and 2, respectively, the polynomial $x_0^2 - x_1$ is homogeneous of degree 2.

This corresponds to a double covering $\sigma : V \rightarrow \mathbb{P}^2$ ramified over the projective curve B .

To have an easy example in mind, consider the affine plane curve C defined by $y^2 = x$, which corresponds to a double covering $\rho : C \rightarrow \mathbb{C}$ of the affine line \mathbb{C} . The zero set of the right-hand side of $y^2 = x$ is given by the one-point set $\{0\} \subset \mathbb{C}$. Notice that the fiber $\rho^{-1}(0)$ is a double point, while for any other $x \neq 0$, it consists of two distinct points. Therefore, we say that $\{0\} \subset \mathbb{C}$ is the *branch locus* and that the covering is *ramified* over $\{0\} \subset \mathbb{C}$.

We write \tilde{V} for the smooth model of V .

One may think of the *smooth model* \tilde{V} as a smoothed version of V that has no singular points. The smooth model is obtained by blowing up all singularities of the original hypersurface. Blow-ups of singularities are always given by birational maps. Thus, a hypersurface is always birational to its smooth model. To learn how to perform blow-ups in practice, we refer the reader to [56].

A necessary condition for \tilde{V} to be rational is that its Kodaira dimension $\text{kod}(\tilde{V})$ is equal to $-\infty$.

The *Kodaira dimension* $\text{kod}(\tilde{V})$ of \tilde{V} is a birational invariant of \tilde{V} . Physicists may think of it as a generalization of the genus notion for higher-dimensional hypersurfaces beyond the case of curves. One can use the Kodaira dimension

to divide algebraic hypersurfaces into several classes. In particular, all rational hypersurfaces have Kodaira dimension $-\infty$.

Since all singularities of the degree- $2k$ curve B are simple, the Kodaira dimension of \tilde{V} is given by

$$\text{kod}(\tilde{V}) = \begin{cases} -\infty, & \text{if } k = 1, 2, \\ 0, & \text{if } k = 3, \\ 2, & \text{if } k \geq 4. \end{cases}$$

These values for $\text{kod}(\tilde{V})$ are derived in Section 22 of Chapter 5 in [85].

Thus, if $k \geq 3$, then \tilde{V} is not rational. Recall that \tilde{V} is birational to V and that V defines *surface* in $\mathbb{P}(k, 1, 1, 1)$, i.e., the notions of uni-rationality and rationality are equivalent for V . Therefore, if $k \geq 3$, then V is not parametrizable by rational functions. \square

In conclusion, the only task to perform in practice is to classify the singularities of a projective curve. In the remaining sections of this chapter, we will explain how to do this in two different manners: on the one hand, we will see that, in special cases, one can classify singularities via elementary geometric arguments. On the other hand, we will show how to use the `ClassSing` function to automatically check for simple singularities. Both methods will be applied to a set of square roots that is relevant for high energy physics.

6.2. CLASSIFICATION OF SINGULARITIES BY GEOMETRIC ARGUMENTS

To get an idea of how to perform the classification of curve singularities in practice, let us discuss an example of physical relevance. In some cases, such as the one at hand, the given set of square roots yields a singularity structure that allows us to deduce the full classification by geometric arguments.

We consider the set of square roots

$$\mathcal{R} = \left\{ \sqrt{x+1}, \sqrt{x-1}, \sqrt{y+1}, \sqrt{x+y+1}, \sqrt{16x + (4+y)^2} \right\},$$

which appears in the computation of certain quantum chromodynamics (QCD) corrections [6], and want to show that this set is not rationalizable. By the results of the previous section, it is sufficient to prove that the projective closure B of the affine degree-6 curve defined by

$$0 = (x+1) \cdot (x-1) \cdot (y+1) \cdot (x+y+1) \cdot (16x + (4+y)^2)$$

has only simple singularities. Notice that the projective curve B is a union of four lines $L_i = \mathbb{V}(l_i) \subset \mathbb{P}^2$, $i = 1, 2, 3, 4$, together with a smooth conic $Q = \mathbb{V}(q) \subset \mathbb{P}^2$. More precisely, we have

$$B = \mathbb{V}(l_1 \cdot l_2 \cdot l_3 \cdot l_4 \cdot q) \subset \mathbb{P}^2$$

with homogeneous polynomials

$$l_1(x, y, z) = x+z, \quad l_2(x, y, z) = x-z, \quad l_3(x, y, z) = y+z, \quad l_4(x, y, z) = x+y+z,$$

and

$$q(x, y, z) = 16xz + (4z+y)^2.$$

Since all components of B define smooth curves themselves, possible singularities of B can only arise from intersection points of these components. The four lines intersect in six points, namely

$$\begin{aligned} L_1 \cap L_2 &= [0 : 1 : 0], \quad L_1 \cap L_3 = [-1 : -1 : 1], \quad L_1 \cap L_4 = [-1 : 0 : 1], \\ L_2 \cap L_3 &= [1 : -1 : 1], \quad L_2 \cap L_4 = [1 : -2 : 1], \quad L_3 \cap L_4 = [0 : -1 : 1]. \end{aligned}$$

Five of these points are intersection points of two lines and, therefore, A_1 singularities of B . The point $[-1 : 0 : 1]$ is, however, an exception. The reason is that $[-1 : 0 : 1]$ is a point of Q , as well. So instead of *two* smooth branches, we see that *three* smooth branches of B pass through this point. It is easy to check that all three branches have different tangent spaces in this point. Therefore, we conclude that $[-1 : 0 : 1]$ is a D_4 singularity. Calculating the intersection points of Q with each line, we obtain

$$\begin{aligned}
L_1 \cap Q &= \{[-1 : 0 : 1], [-1 : -8 : 1]\}, \\
L_2 \cap Q &= \{[1 : -4 - 4i : 1], [1 : -4 + 4i : 1]\}, \\
L_3 \cap Q &= \{[1 : 0 : 0], [-9/16 : -1 : 1]\}, \\
L_4 \cap Q &= \{[-1 : 0 : 1], [-9 : 8 : 1]\}.
\end{aligned}$$

Except $[-1 : 0 : 1]$, all of these points are again intersections of two smooth branches with different tangent spaces in the respective point.

In summary, the singular locus of B is given by eleven A_1 and a single D_4 singularity. In particular, all singularities of B are simple, and we can conclude that the set \mathcal{R} is not rationalizable.

6.3. THE CLASSSING FUNCTION

We can also perform the singularity classification in an automated fashion with **Magma**. For this purpose, we will use the **ClassSing** function, which was developed in joint work with Dino Festi [4]. The latest version is available at the author's GitHub repository [52].

The function is executed with the following command:

```
> ClassSing(basering, polynomial);
```

Its first input is the ring of polynomials in three variables $K[x, y, z]$, where K is a field. Let us stress that the user always has to use the letters x , y , and z for the variable names. The second input is the homogeneous polynomial that defines the projective curve whose singularities we want to study. The output is a string that tells the user whether all singularities of the given projective curve are ADE singularities.

Internally, **ClassSing** examines three affine surfaces. Each of these surfaces corresponds to one of the affine charts of the input curve. Subsequently, **ClassSing** calls the **Magma** function **HasOnlySimpleSingularities**. The output of this

function is then used to draw conclusions on the singularity structure of the input curve.

To see how `ClassSing` is to be applied in practice, let us consider the set of square roots \mathcal{R} of the previous section. Recall that, in order to show non-rationalizability of \mathcal{R} , we need to prove that all singularities of the projective curve

$$B = \mathbb{V}((x+z)(x-z)(y+z)(x+y+z)(16xz + (4z+y)^2)) \subset \mathbb{P}^2$$

are ADE singularities.

Before we can use `ClassSing`, there is one important subtlety that we have to address. As we have already seen, not all singular points of B have rational coordinates. This is problematic, because `Magma` will not allow us to choose $K = \mathbb{C}$ for our base ring $K[x, y, z]$. It does, however, allow us to choose the field of rational numbers $K = \mathbb{Q}$. But if we would determine the singular points of B with this choice of base ring, it would only give us the singular points of B that have purely rational coordinates, i.e., we would overlook two of the singular points of B in our analysis.

To resolve this issue, we first compute the singular points with a different computer algebra software that will not only be sensitive to singularities over \mathbb{Q} but to all singular points over \mathbb{C} . For example, we can compute the singular points of B in `Mathematica` via

```
> f := (x + z)*(x - z)*(y + z)*(x + y + z)*(16*x*z + (4*z + y)^2)
> Solve[f == 0 && D[f, x] == 0 && D[f, y] == 0 && D[f, z] == 0]
```

giving us the output

```
{ {x -> -z, y -> 0}, {x -> -z, y -> -8 z}, {x -> -z, y -> -z},
  {x -> z, y -> (-4 - 4 i) z}, {x -> z, y -> (-4 + 4 i) z},
  {x -> z, y -> -2 z}, {x -> z, y -> -z}, {x -> -z, y -> 0},
  {x -> -((9 z)/16), y -> -z}, {x -> -9 z, y -> 8 z},
```

```
{x -> 0, z -> 0}, {y -> 0, z -> 0}, {x -> 0, y -> -z},  
{x -> 0, y -> 0, z -> 0}}
```

which corresponds to the 12 singular points that we already determined in the previous section. Notice that we ignore the trivial solution, since $[0 : 0 : 0]$ is not an element of \mathbb{P}^2 . From the **Mathematica** output, we see that two of the singular points have irrational numbers in their coordinates. Now that we know the exact irrationalities in the coordinates of the singular points, we can perform the remaining analysis in **Magma**.

In order for **ClassSing** to be able to consider all of the singular points of B , we have to adjoin the imaginary unit to the coefficient field \mathbb{Q} of our base ring $\mathbb{Q}[x, y, z]$. Put differently, we have to pass from \mathbb{Q} to the extension field $\mathbb{Q}(\sqrt{-1})$. A convenient way to construct an extension field for \mathbb{Q} is to consider a quotient ring of the polynomial ring $\mathbb{Q}[x]$ that corresponds to the irrational numbers we want to be contained in the extension field. In our example, \mathbb{Q} does not contain the imaginary unit i , i.e., it does not contain any element x with $x^2 + 1 = 0$. The sought-after extension field $\mathbb{Q}(\sqrt{-1})$ is, therefore, to be constructed as the quotient ring $\mathbb{Q}(\sqrt{-1}) = \mathbb{Q}[x]/(x^2 + 1)$. In **Magma**, $\mathbb{Q}(\sqrt{-1})$ is easily defined via

```
> QQ:=Rationals();  
> F<i>:=ext<QQ| [Polynomial([1,0,1])]>;
```

where **Polynomial([1,0,1])** specifies the coefficients of the polynomial g in the quotient $\mathbb{Q}[x]/g$, in our case $g = 1 \cdot x^0 + 0 \cdot x^1 + 1 \cdot x^2$.

If the coordinates of the singular points under consideration would contain more than one irrationality, for instance the imaginary unit i and, in addition, the irrational number $a := \sqrt{5}$, then the corresponding field extension $\mathbb{Q}(\sqrt{5}, \sqrt{-1})$ can be created via

```
> QQ:=Rationals();  
> F<i,a>:=ext<QQ| [Polynomial([1,0,1]), Polynomial([-5,0,1])]>;
```

Now, we can easily prove the non-rationalizability of \mathcal{R} using `ClassSing`:

```
> QQ:=Rationals();
> F<i>:=ext<QQ|[Polynomial([1,0,1])]>;
> K<x,y,z>:=PolynomialRing(F,3);
> f:=(x+z)*(x-z)*(y+z)*(x+y+z)*(16*x*z+(4*z+y)^2);
> ClassSing(K,f);
All singularities of the given projective curve
are ADE singularities.
```

6.4. SETS OF SQUARE ROOTS BEYOND Two VARIABLES

To conclude Part 2, let us give some final comments on how the presented techniques may be applied beyond the case of two variables. As already mentioned in Chapter 1, a general treatment of the case in three or more variables will immediately lead us to the edge of knowledge of contemporary mathematics since the relevant hypersurfaces are no longer given by curves or surfaces. Nevertheless, even the cases of square roots in one and two variables are already relevant for a large number of modern physics applications.

Further, the reader should bear in mind that it is sufficient to prove non-rationalizability for a *subset* of square roots. So even in the case of large sets, one might be able to find a subset that consists only of square roots whose non-rationalizability can be proven by our techniques. Also, we want to point out that the theorem at the beginning of the present chapter applies naturally to sets of square roots in *three* variables, whenever there exists a subset of square roots whose arguments are all given by *homogeneous* polynomials.

In conclusion, our methods can also be useful beyond the case of two variables as long as the given set of square roots has a subset that depends on at most two variables or may consist of square roots in three variables whose arguments are all homogeneous polynomials.

Part 3

Rationalization Techniques

CHAPTER 7

The Main Rationalization Algorithm

In this final part of the thesis, we will give a detailed discussion on how one can rationalize a given set of square roots. The presented algorithm is based on the parametrization by lines method—a technique well-known in the theory of curves and surfaces—and generalizes this method to the case of hypersurfaces of dimension $n \in \mathbb{N}$. We will see that the algorithm is applicable whenever the degree- d hypersurface under consideration has a point of multiplicity $d - 1$. Then, considering a family of lines through this $(d - 1)$ -point, this family will intersect the hypersurface in only a single other point whose coordinates we can use as a rational parametrization. In this way, we can always find a rational parametrization algorithmically as soon as the given hypersurface has a $(d - 1)$ -point.

7.1. INTRODUCTORY EXAMPLES

Consider a square root $\sqrt{p/q}$ of a rational function, where $p, q \in \mathbb{C}[x_1, \dots, x_n]$ are polynomials. We associate a hypersurface to this square root by naming it, e.g., denote it by r , squaring the resulting equation, and clearing the denominator. More precisely, we define the *associated hypersurface* of $\sqrt{p/q}$ as the affine hypersurface given by $V = \mathbb{V}(q \cdot r^2 - p) \subset \mathbb{C}^{n+1}$.

Notice that we can also associate a hypersurface to more general algebraic functions such as roots of degree greater than 2 or nested roots. For example, $V = \mathbb{V}(r^3 - x^3 - x^2)$ is associated to $\sqrt[3]{x^3 + x^2}$ and

$$W = \mathbb{V}((r^2 - x^2)^2 - x^4 - y^3)$$

is associated to

$$\sqrt{x^2 + \sqrt{x^4 + y^3}}.$$

To clarify the idea behind the rationalization algorithm, we will devote this introductory section to the simple case of square roots in a single variable so that the associated hypersurfaces are always given by curves.

Example Suppose we want to rationalize the square root $\sqrt{x^3 + x^2}$. Its associated hypersurface is the nodal cubic $V = \mathbb{V}(r^2 - x^3 - x^2)$. We have already seen in Part 1 that a degree-3 curve is parametrizable by rational functions if it has an ordinary double point.

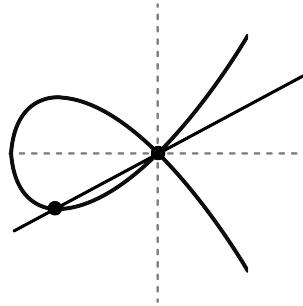


FIGURE 7.1. Parametrizing the nodal cubic by a family of lines.

In fact, we can parametrize the nodal cubic similarly to the circle by intersecting it with a family of lines: if we consider a family of lines $r = tx$ through the singular point, then each member of this family will intersect the curve in only a single other point whose coordinates provide the sought-after parametrization $(\phi_r(t), \phi_x(t)) = (t(t^2 - 1), t^2 - 1)$. Finally, we can use this parametrization to rationalize $\sqrt{x^3 + x^2}$:

$$\sqrt{\phi_x^3(t) + \phi_x^2(t)} = t(t^2 - 1).$$

◊

The most important thing that the reader should take away from this example is that it is precisely the fact that the nodal cubic has a point of multiplicity 2, which allows us to parametrize the curve by a family of lines. More generally, we can always parametrize a given degree- d hypersurface through lines whenever it

has at least one $(d - 1)$ -point. This is easiest to see through another example. Let us, therefore, consider the case of the unit circle one more time.

Example We have already seen how to construct the parametrization of the unit circle geometrically. Let us now go through the same construction again, but in a more algebraic manner. In order to determine a rational parametrization of $V = \mathbb{V}(f) = \mathbb{V}(x^2 + y^2 - 1)$, we need to find a $(d - 1)$ -point. Because the degree of V is given by $d = \deg(V) = 2$, we may choose any regular point of V , e.g., $p_0 = (x_0, y_0) = (-1, 0) \in V$. Next, we translate p_0 to the origin, i.e., we send $x \mapsto x + 1$ and $y \mapsto y$. The polynomial f becomes

$$f(x, y) = f_1(x, y) + f_2(x, y)$$

with homogeneous components

$$f_1(x, y) = -2x \text{ and } f_2(x, y) = x^2 + y^2$$

of degree 1 and 2, respectively. Now, consider a family of lines $y = tx$ through p_0 . We determine the two intersection points of each of the lines with the circle by plugging the line equation into $f(x, y) = 0$:

$$0 = f_1(x, tx) + f_2(x, tx) = xf_1(1, t) + x^2f_2(1, t).$$

The solution $x = 0$ gives p_0 . The second solution yields

$$x = -\frac{f_1(1, t)}{f_2(1, t)}, \quad y = -t\frac{f_1(1, t)}{f_2(1, t)}.$$

Translating back to the original setting via $x \mapsto x - 1$ and $y \mapsto y$, we see that

$$\phi_x(t) = -\frac{f_1(1, t)}{f_2(1, t)} - 1, \quad \phi_y(t) = -t\frac{f_1(1, t)}{f_2(1, t)},$$

yields the sought-after parametrization. Notice that we had a choice in picking the family of lines through p_0 which we intersected with the circle. In fact, one can easily produce a different rational parametrization by considering a different family of lines. For instance, taking the family to be $x = ty$ instead, we find the parametrization

$$\phi_x(t) = -t\frac{f_1(t, 1)}{f_2(t, 1)} - 1, \quad \phi_y(t) = -\frac{f_1(t, 1)}{f_2(t, 1)}.$$

This brings us to the main algorithm that we will use for our rationalizations.

7.2. THE ALGORITHM

Input A degree- d hypersurface V that is associated to a given root, and whose projective closure \bar{V} has at least one point of multiplicity $d - 1$.

Output A rational parametrization of V .

1. Determine a point p_0 with $\text{mult}_{p_0} V = d - 1$.
2. If p_0 is *not* at infinity, continue with step 3. and 4., and finish with step 5.
If p_0 is at infinity, consider another affine chart V' of the projective closure \bar{V} in which p_0 is not a point at infinity, continue with steps 3., 4., 5., and finish with step 6.
3. With $p_0 = (a_0, \dots, a_n)$, compute

$$g(r, x_1, \dots, x_n) = f(r + a_0, x_1 + a_1, \dots, x_n + a_n),$$

and write

$$g(r, x_1, \dots, x_n) = g_d(r, x_1, \dots, x_n) + g_{d-1}(r, x_1, \dots, x_n),$$

where g_d and g_{d-1} are homogeneous components of degree d and $d - 1$.

4. Return

$$\begin{aligned} \phi_r(t_0, \dots, t_n) &= -t_0 \frac{g_{d-1}(t_0, t_1, \dots, t_n)}{g_d(t_0, t_1, \dots, t_n)} + a_0, \\ &\vdots \\ \phi_{x_n}(t_1, \dots, t_n) &= -t_n \frac{g_{d-1}(t_0, t_1, \dots, t_n)}{g_d(t_0, t_1, \dots, t_n)} + a_n. \end{aligned}$$

5. For a single $i \in \{0, \dots, n\}$, set $t_i = 1$.
6. Change coordinates, to switch from V' to the original affine chart V .

7.3. SAMPLE APPLICATIONS

Example As a first example, let us apply the algorithm to rationalize the square root $\sqrt{1 - x^2}$ with associated hypersurface $V = \mathbb{V}(r^2 + x^2 - 1) \subset \mathbb{C}^2$.

Step 1. Because $\deg(V) = 2$, we can use any regular point of V as our point of multiplicity $d - 1$. For instance, choose $p_0 = (r_0, x_0) = (0, -1)$.

Step 2. p_0 is not a point at infinity.

Step 3. Consider $g(r, x) = f(r + 0, x + (-1)) = g_2(r, x) + g_1(r, x)$, where $g_2(r, x) = r^2 + x^2$ and $g_1(r, x) = -2x$.

Step 4. Return

$$\begin{aligned}\phi_r(t_0, t_1) &= -t_0 \frac{g_1(t_0, t_1)}{g_2(t_0, t_1)} + 0, \\ \phi_x(t_0, t_1) &= -t_1 \frac{g_1(t_0, t_1)}{g_2(t_0, t_1)} + (-1).\end{aligned}$$

Step 5. Setting $t_0 = 1$ we obtain

$$\begin{aligned}\phi_r(t_1) &:= \phi_r(1, t_1) = -\frac{g_1(1, t_1)}{g_2(1, t_1)} = \frac{2t_1}{t_1^2 + 1}, \\ \phi_x(t_1) &:= \phi_x(1, t_1) = -t_1 \frac{g_1(1, t_1)}{g_2(1, t_1)} - 1 = \frac{t_1^2 - 1}{t_1^2 + 1},\end{aligned}$$

and $\phi_x(t_1)$ provides a substitution that rationalizes $\sqrt{1 - x^2}$.

Example Let us proceed with a more involved example. Consider the square root

$$\sqrt{\frac{x^4 + 4x^2y^2 + 4}{4x^2}}.$$

The associated hypersurface is $V = \mathbb{V}(f) = \mathbb{V}(x^4 + 4x^2y^2 + 4 - 4r^2x^2)$.

Step 1. Because $\deg(V) = 4$, we need a point of multiplicity 3 to apply the algorithm. Looking at the partial derivatives of f , we see that V does not have such a point. There is, however, a point of multiplicity 3 at infinity as we can see by considering the projective closure

$$\bar{V} = \mathbb{V}(x^4 + 4x^2y^2 + 4z^4 - 4r^2x^2).$$

This $(d-1)$ -point is given by $p_0 = [r_0 : x_0 : y_0 : z_0] = [1 : 0 : 1 : 0]$.

Step 2. Viewed from the affine chart V , p_0 is at infinity. Therefore, we have to consider a different affine chart V' of \bar{V} for which p_0 is not at infinity. In this particular example, we have two choices: either we consider the chart in which $r = 1$ or the chart in which $y = 1$. Let us choose the former, which corresponds to a map

$$[r : x : y : z] \mapsto \left(\frac{x}{r}, \frac{y}{r}, \frac{z}{r} \right) =: (x', y', z').$$

Under this mapping, $p_0 \in \bar{V}$ is send to $p'_0 := (0, 1, 0) \in V'$. The affine hypersurface V' is given by $V' = \mathbb{V}((x')^4 + 4(x')^2(y')^2 + 4(z')^4 - 4(x')^2)$.

Step 3. Consider $g(x', y', z') = f(x'+0, y'+1, z'+0) = g_4(x', y', z') + g_3(x', y', z')$, where $g_4(x', y', z') = (x')^4 + 4(z')^4 + 4(x')^2(y')^2$ and $g_3(x', y', z') = 8(x')^2y'$.

Step 4. Return

$$\begin{aligned} \phi_{x'}(t_0, t_1, t_2) &= -t_0 \frac{g_3(t_0, t_1, t_2)}{g_4(t_0, t_1, t_2)} + 0, \\ \phi_{y'}(t_0, t_1, t_2) &= -t_1 \frac{g_3(t_0, t_1, t_2)}{g_4(t_0, t_1, t_2)} + 1, \\ \phi_{z'}(t_0, t_1, t_2) &= -t_2 \frac{g_3(t_0, t_1, t_2)}{g_4(t_0, t_1, t_2)} + 0. \end{aligned}$$

Step 5. Setting $t_0 = 1$ we obtain

$$\begin{aligned}\phi_{x'}(t_1, t_2) &:= \phi_{x'}(1, t_1, t_2) = -\frac{g_3(1, t_1, t_2)}{g_4(1, t_1, t_2)} = -\frac{8t_1}{4t_2^4 + 4t_1^2 + 1}, \\ \phi_{y'}(t_1, t_2) &:= \phi_{y'}(1, t_1, t_2) = -t_1 \frac{g_3(1, t_1, t_2)}{g_4(1, t_1, t_2)} + 1 = \frac{4t_2^4 - 4t_1^2 + 1}{4t_2^4 + 4t_1^2 + 1}, \\ \phi_{z'}(t_1, t_2) &:= \phi_{z'}(1, t_1, t_2) = -t_2 \frac{g_3(1, t_1, t_2)}{g_4(1, t_1, t_2)} = -\frac{8t_1 t_2}{4t_2^4 + 4t_1^2 + 1}.\end{aligned}$$

Step 6. Finally, we use the parametrization for V' to construct a parametrization for V . More precisely, we solve

$$\phi_{x'} = \frac{\phi_x}{\phi_r}, \quad \phi_{y'} = \frac{\phi_y}{\phi_r}, \quad \text{and} \quad \phi_{z'} = \frac{\phi_z}{\phi_r}$$

for ϕ_r , ϕ_x , and ϕ_y while putting $\phi_z = 1$. We find that the sought-after substitutions are given by

$$\begin{aligned}\phi_x(t_1, t_2) &= \frac{1}{t_2}, \\ \phi_y(t_1, t_2) &= -\frac{4t_2^4 - 4t_1^2 + 1}{8t_1 t_2},\end{aligned}$$

and can easily check that they rationalize our square root:

$$\sqrt{\frac{(\phi_x(t_1, t_2))^4 + 4(\phi_x(t_1, t_2))^2(\phi_y(t_1, t_2))^2 + 4}{4(\phi_x(t_1, t_2))^2}} = \frac{4t_2^4 + 4t_1^2 + 1}{8t_1 t_2}.$$

7.4. SIMULTANEOUS RATIONALIZATION OF MULTIPLE SQUARE ROOTS

Now that we have seen how to rationalize individual square roots, let us demonstrate how to find a variable change that rationalizes a whole set of square roots. Consider the set

$$\mathcal{R} = \left\{ \sqrt{x+1}, \sqrt{x-1}, \sqrt{y+1}, \sqrt{x+y+1} \right\}$$

whose rationalization is relevant in the computation of certain QCD corrections [6]. In fact, this set is a rationalizable subset of the non-rationalizable set that we have studied in Part 2.

Our strategy will be to rationalize one square root at a time in an iterative manner. More precisely, we first choose one of the square roots as our starting point and apply our rationalization algorithm to this square root. While the resulting substitution will rationalize this particular square root, it will not rationalize the remaining ones. Instead, it will affect all of the other square root arguments that depend on the variable that we have changed. This will leave us with a new set of square roots with more complicated square root arguments. In particular, these new arguments will, in general, be rational functions rather than polynomials. Nevertheless, this new set of square roots will contain one element less. Therefore, we may repeat this procedure until all square roots are rationalized. Finally, the composition of all the variable changes that we have found will give us a single variable change that rationalizes all of the given square roots simultaneously.

To clarify this procedure, let us present the rationalization of \mathcal{R} in detail.

Step 1: Rationalizing $\sqrt{x+1}$

The associated hypersurface of $\sqrt{x+1}$ is the conic plane curve $V_1 = \mathbb{V}(r_1^2 - x - 1)$. Since $\deg(V_1) = 2$, any regular point p_1 of V_1 is a $(d-1)$ -point. For instance, we apply the algorithm with the choice $p_1 = (0, -1)$, which yields the following rational parametrization of V_1 :

$$(\phi_{r_1}(t_1), \phi_x(t_1)) = \left(\frac{1}{t_1}, \frac{1 - t_1^2}{t_1^2} \right).$$

Admittedly, this parametrization is more complicated than it needs to be since the substitution $x = t_1^2 - 1$ would also rationalize the square root. However, this choice would lead to more complicated coefficients in a later step, which is why we stick with the parametrization above.

Step 2: Rationalizing $\sqrt{x-1}$

Next, we want to find a substitution which rationalizes $\sqrt{x-1}$. At the same time, we have to guarantee that this new substitution, which we denote by $\varphi_x(t_2)$, also rationalizes the first square root $\sqrt{x+1}$. To achieve this, we first substitute $\phi_x(t_1)$ in the square root $\sqrt{x-1}$:

$$\sqrt{\phi_x(t_1) - 1} = \sqrt{\frac{1 - 2t_1^2}{t_1^2}}.$$

Since the denominator of the right-hand side is already a square, we just need to rationalize the square root of the numerator. We should stress, though, that excluding square factors from the analysis is not always beneficial. We will discuss the role of squares in more detail in one of the upcoming chapters.

For now, notice that the associated hypersurface of our new square root $\sqrt{1 - 2t_1^2}$ is given by $V_2 = \mathbb{V}(r_2^2 + 2t_1^2 - 1)$. Again, since $\deg(V_2) = 2$, any regular point p_2 of V_2 is a $(d - 1)$ -point. For instance, we may choose $p_2 = (1, 0)$. Applying the algorithm with this choice yields the parametrization

$$(\phi_{r_2}(t_2), \phi_{t_1}(t_2)) = \left(1 - \frac{2t_2^2}{t_2^2 + 2}, -\frac{2t_2}{t_2^2 + 2}\right).$$

We can now write down the expression for $\varphi_x(t_2)$ by composing the two substitutions that rationalize the individual square roots:

$$\varphi_x(t_2) := \phi_x(\phi_{t_1}(t_2)) = \frac{t_2^4 + 4}{4t_2^2}.$$

Indeed, we can check that plugging $\varphi_x(t_2)$ into $\sqrt{x+1}$ and $\sqrt{x-1}$ yields rational expressions:

$$\begin{aligned}\sqrt{\varphi_x(t_2) + 1} &= \frac{t_2^2 + 2}{2t_2}, \\ \sqrt{\varphi_x(t_2) - 1} &= \frac{t_2^2 - 2}{2t_2}.\end{aligned}$$

Step 3: Rationalizing $\sqrt{y+1}$

In principle, we could rationalize $\sqrt{y+1}$ similarly to $\sqrt{x+1}$, i.e., we could simply replace y by $(1 - t_3^2)/t_3^2$. However, this substitution would yield a rather complicated hypersurface when we try to rationalize $\sqrt{x+y+1}$ in the upcoming step. So in the case at hand, it is better to take the obvious choice

$$\varphi_y(t_3) = t_3^2 - 1.$$

Step 4: Rationalizing $\sqrt{x+y+1}$

We have seen that the first three square roots of \mathcal{R} can be rationalized with the substitutions

$$\begin{aligned}\varphi_x(t_2) &= \frac{t_2^4 + 4}{4t_2^2}, \\ \varphi_y(t_3) &= t_3^2 - 1.\end{aligned}$$

Plugging these expressions into the remaining square root $\sqrt{x+y+1}$, we obtain

$$\sqrt{\frac{t_2^4 + 4t_2^2t_3^2 + 4}{4t_2^2}}.$$

The associated hypersurface is given by $V_4 = \mathbb{V}(t_2^4 + 4t_2^2t_3^2 + 4 - 4r_4^2t_2^2)$. Notice that this is precisely the hypersurface that we studied in the second example of the previous section. A rational parametrization of V_4 is, therefore, given by the three rational functions

$$\begin{aligned}\phi_{r_4}(s_1, s_2) &= -\frac{4s_2^4 + 4s_1^2 + 1}{8s_1s_2}, \\ \phi_{t_2}(s_1, s_2) &= \frac{1}{s_2}, \\ \phi_{t_3}(s_1, s_2) &= -\frac{4s_2^4 - 4s_1^2 + 1}{8s_1s_2}.\end{aligned}$$

Finally, composing these functions with the ones that rationalize the other square roots, we obtain substitutions that rationalize all of the four square roots in \mathcal{R} simultaneously:

$$\begin{aligned}\Phi_x(s_1, s_2) &:= \varphi_x(\phi_{t_2}(s_1, s_2)), \\ \Phi_y(s_1, s_2) &:= \varphi_y(\phi_{t_3}(s_1, s_2)).\end{aligned}$$

Indeed, we find that

$$\begin{aligned}\sqrt{\Phi_x(s_1, s_2) + 1} &= \frac{2s_2^2 + 1}{2s_2}, \\ \sqrt{\Phi_x(s_1, s_2) - 1} &= \frac{2s_2^2 - 1}{2s_2}, \\ \sqrt{\Phi_y(s_1, s_2) + 1} &= \frac{4s_2^4 - 4s_1^2 + 1}{8s_1s_2}, \\ \sqrt{\Phi_x(s_1, s_2) + \Phi_y(s_1, s_2) + 1} &= \frac{4s_2^4 + 4s_1^2 + 1}{8s_1s_2}.\end{aligned}$$

CHAPTER 8

The F-Decomposition Theorem

Now that we have a good understanding of the standard machinery, let us turn to a more advanced technique. In the following chapter, we will present the F -decomposition theorem, which was first proved by the author in the appendix of [3] and turned out to be a useful tool in many applications. In fact, it often allows for rationalizations that would otherwise be out of reach.

8.1. THE THEOREM

If k is a positive integer and $f \in \mathbb{C}[x_1, \dots, x_n]$ a polynomial of degree d with $d \leq k$, then the k -homogenization of f is a degree- k homogeneous polynomial

$$F(x_1, \dots, x_n, z) := z^k \cdot f(x_1/z, \dots, x_n/z).$$

For example, the 4-homogenization of $f(x, y) = xy$ is given by $F(x, y, z) = xyz^2$. The d -homogenization of a degree- d polynomial is the usual homogenization.

Theorem (F-Decomposition Theorem) If $V = \mathbb{V}(r^2 - f_{\frac{d}{2}}^2 + 4f_{\frac{d}{2}+1}f_{\frac{d}{2}-1}) \subset \mathbb{C}^{n+1}$ denotes the hypersurface associated to

$$\sqrt{f_{\frac{d}{2}}^2 - 4f_{\frac{d}{2}+1}f_{\frac{d}{2}-1}},$$

where each $f_k \in \mathbb{C}[x_1, \dots, x_n]$ is a polynomial of degree $\deg(f_k) \leq k$, then V has a rational parametrization if and only if $W = \mathbb{V}(F_{\frac{d}{2}+1} + F_{\frac{d}{2}} + F_{\frac{d}{2}-1}) \subset \mathbb{C}^{n+1}$ has a rational parametrization with F_k being the k -homogenization of f_k using the same homogenizing variable, say z , for each of the three homogenizations.

Proof If $(\phi_{x_1}^W, \dots, \phi_{x_n}^W, \phi_z^W)$ is a rational parametrization of W , then we obtain a rational parametrization of V by defining

$$\begin{aligned}
\phi_r^V &:= 2 \cdot \phi_z^W \cdot f_{\frac{d}{2}+1}(\phi_{x_1}^W/\phi_z^W, \dots, \phi_{x_n}^W/\phi_z^W) + f_{\frac{d}{2}}(\phi_{x_1}^W/\phi_z^W, \dots, \phi_{x_n}^W/\phi_z^W), \\
\phi_{x_1}^V &:= \frac{\phi_{x_1}^W}{\phi_z^W}, \\
&\vdots \\
\phi_{x_n}^V &:= \frac{\phi_{x_n}^W}{\phi_z^W}.
\end{aligned}$$

For the converse direction, which we will not use in this thesis, we refer the reader to the original paper [3]. \square

8.2. SAMPLE APPLICATION

To see how useful the F -decomposition theorem is in practice, let us discuss a rationalization that uses all of the techniques discussed so far.

Consider the square root $\sqrt{x^4 + y^3}$. The associated affine hypersurface reads $V = \mathbb{V}(f) = \mathbb{V}(r^2 - x^4 - y^3)$. Because V has degree 4, we need to find a point p of multiplicity 3 to apply the rationalization algorithm. Computing the partial derivatives of the homogenization of f , however, we see that V does not have a point of multiplicity 3—not even at infinity. Let us, therefore, apply the F -decomposition theorem:

First, we observe that

$$\sqrt{x^4 + y^3} = \sqrt{f_2^2 - 4f_3f_1}$$

with

$$f_1(x, y) = -\frac{1}{4}, \quad f_2(x, y) = x^2, \quad f_3(x, y) = y^3,$$

and corresponding k -homogenizations

$$F_1(x, y, z) = -\frac{1}{4}z, \quad F_2(x, y, z) = x^2, \quad F_3(x, y, z) = y^3.$$

According to the theorem, V has a rational parametrization if the hypersurface

$$W = \mathbb{V}(F_1 + F_2 + F_3) = \mathbb{V}(-z/4 + x^2 + y^3) \subset \mathbb{C}^3$$

has a rational parametrization. Thus, we try to apply the algorithm to W :

Step 1. Because $\deg(W) = 3$, we need to find a point of multiplicity 2. Looking at the partial derivatives of $F_1 + F_2 + F_3$, we see that W does not have such a point. There is, however, a point of multiplicity 2 at infinity. We see this by considering the projective closure

$$\bar{W} = \mathbb{V}(v^2 F_1 + v F_2 + F_3) \subset \mathbb{P}^3.$$

This projective hypersurface has a single point of multiplicity 2, namely

$$p_0 = [x_0 : y_0 : z_0 : v_0] = [0 : 0 : 1 : 0].$$

Step 2. Viewed from the affine chart W , p_0 is at infinity because v_0 is zero. Therefore, we have to consider a different affine chart W' of \bar{W} in which p_0 is not at infinity. In this particular example, we only have one choice, namely to consider the chart where $z = 1$. Switching from \bar{W} to W' corresponds to a map

$$[x : y : z : v] \mapsto (x/z, y/z, v/z) =: (x', y', v').$$

Under this mapping, $p_0 \in \bar{W}$ is sent to $p'_0 := (0, 0, 0) \in W'$. The affine hypersurface W' is given by

$$W' = \mathbb{V}\left(-(v')^2/4 + v'(x')^2 + (y')^3\right) \subset \mathbb{C}^3.$$

Step 3. Consider

$$\begin{aligned} g(x', y', v') &= -(v' + 0)^2/4 + (v' + 0)(x' + 0)^2 + (y' + 0)^3 \\ &= g_3(x', y', v') + g_2(x', y', v'), \end{aligned}$$

where

$$g_3(x', y', v') = v'(x')^2 + (y')^3 \text{ and } g_2(x', y', v') = -(v')^2/4.$$

Step 4. Return

$$\begin{aligned}\phi_{x'}(t_0, t_1, t_2) &= -t_0 \frac{g_2(t_0, t_1, t_2)}{g_3(t_0, t_1, t_2)} + 0, \\ \phi_{y'}(t_0, t_1, t_2) &= -t_1 \frac{g_2(t_0, t_1, t_2)}{g_3(t_0, t_1, t_2)} + 0, \\ \phi_{v'}(t_0, t_1, t_2) &= -t_2 \frac{g_2(t_0, t_1, t_2)}{g_3(t_0, t_1, t_2)} + 0.\end{aligned}$$

Step 5. Setting $t_0 = 1$, we obtain

$$\begin{aligned}\phi_{x'}(t_1, t_2) &:= \phi_{x'}(1, t_1, t_2) = -\frac{g_2(1, t_1, t_2)}{g_3(1, t_1, t_2)} = \frac{t_2^2}{4(t_1^3 + t_2)}, \\ \phi_{y'}(t_1, t_2) &:= \phi_{y'}(1, t_1, t_2) = -t_1 \frac{g_2(1, t_1, t_2)}{g_3(1, t_1, t_2)} = \frac{t_1 t_2^2}{4(t_1^3 + t_2)}, \\ \phi_{v'}(t_1, t_2) &:= \phi_{v'}(1, t_1, t_2) = -t_2 \frac{g_3(1, t_1, t_2)}{g_4(1, t_1, t_2)} = \frac{t_2^3}{4(t_1^3 + t_2)}.\end{aligned}$$

Step 6. The next step is to translate the rational parametrization for W' into a rational parametrization for W . To do this, we solve

$$\phi_{x'} = \frac{\phi_x}{\phi_z}, \quad \phi_{y'} = \frac{\phi_y}{\phi_z}, \quad \text{and} \quad \phi_{v'} = \frac{\phi_v}{\phi_z}$$

for ϕ_x , ϕ_y , and ϕ_z while putting $\phi_v = 1$. In this way, we obtain a rational parametrization of W as

$$\begin{aligned}\phi_x^W(t_1, t_2) &= \frac{1}{t_2}, \\ \phi_y^W(t_1, t_2) &= \frac{t_1}{t_2}, \\ \phi_z^W(t_1, t_2) &= \frac{4(t_1^3 + t_2)}{t_2^3}.\end{aligned}$$

Finally, we use the F -decomposition theorem to obtain the change of variables that rationalizes $\sqrt{x^4 + y^3}$:

$$\begin{aligned}\phi_x^V(t_1, t_2) &= \frac{\phi_x^W(t_1, t_2)}{\phi_z^W(t_1, t_2)} = \frac{t_2^2}{4(t_1^3 + t_2)}, \\ \phi_y^V(t_1, t_2) &= \frac{\phi_y^W(t_1, t_2)}{\phi_z^W(t_1, t_2)} = \frac{t_1 t_2^2}{4(t_1^3 + t_2)}.\end{aligned}$$

Indeed, we have

$$\sqrt{(\phi_x^V(t_1, t_2))^4 + (\phi_y^V(t_1, t_2))^3} = \frac{t_2^3(2t_1^3 + t_2)}{16(t_1^3 + t_2)^2}.$$

CHAPTER 9

The RationalizeRoots Software

The **RationalizeRoots** software package implements all of the techniques that we discussed in the two previous chapters and is the result of joint work with Pascal Wasser and Stefan Weinzierl. The package comes in two versions: one for **Mathematica** and one for **Maple**. In this thesis, we will focus on the **Mathematica** version of the package. For the corresponding **Maple** commands, we refer the reader to the original paper [1].

9.1. SETUP AND DOCUMENTATION

In this first section, we will give a brief overview of the functions of the package and their basic options.

The package is loaded with the command:

```
Get["RationalizeRoots.m"]
```

Once loaded, it provides the following routines:

- **ParametrizePolynomial**[*poly*, *options*]
 - The input *poly* is a (multivariate) polynomial.
 - The output is a list of rational parametrizations for the hypersurface defined by *poly*. Each rational parametrization is given as a substitution list. By default, only one rational parametrization is returned. If no rational parametrization is found, the empty list is returned.
 - Basic Options:
 - * **Variables** → {*x*₁, *x*₂, ...}: Only the variables appearing in the list are considered as variables of *poly*. In case this

option is not specified, all variables appearing in `poly` are taken into account.

- * **OutputVariables** → $\{y_1, y_2, \dots\}$: The variables appearing in the list are used as new variables, i.e., as parameters of the rational parametrization. By default, $t[1]$, $t[2]$, ... are used as new variables.
- * **MultipleSolutions** → `True` / `False`: If true, a list of multiple rational parametrizations is returned. If false, the first rational parametrization found is returned. The default value is `false`.
- * **GeneralC** → `True` / `False`: If true, the rational parametrization may depend on free parameters $C[1]$, $C[2]$, ... If false, a default value is substituted for all occurring free parameters. The default value of the option is `false`.
- * **GeneralT** → `True` / `False`: If true, the option skips step 5 of the rationalization algorithm and leaves it to the user to set one of the new variables equal to one. The default value is `false`.
- * **ForceFDecomposition** → `True` / `False`: If true, the F -decomposition theorem is applied before searching for $(d-1)$ -points on the original hypersurface. The default value is `false`.
- * **FPolynomials** → $\{f_1, f_2, f_3\}$: Given the list $\{f_1, f_2, f_3\}$, assume that `poly` is of the form $r^2 - f_2^2 + 4f_1f_3$ and use these polynomials for the F -decomposition theorem. If this option is not specified, a heuristic algorithm is used to find an F -decomposition.

- **RationalizeRoot** [root, options]

- The input `root` is of the form $R_1\sqrt{R_2}$, where R_1 and R_2 are (multivariate) rational functions.
- The output is a list of variable changes that rationalize the given square root. Each variable change is given as a substitution list. By default, only one variable change is returned. If no variable change is found, the empty list is returned.
- Basic Options:

- * **Variables**: As above.
- * **OutputVariables**: As above.
- * **MultipleSolutions**: As above.
- * **GeneralC**: As above.
- * **GeneralT**: As above.
- * **ForceFDecomposition**: As above.
- * **FPolynomials**: As above, but with the restriction that the input is assumed to be a square root of a polynomial P , which can be written as $\sqrt{P} = \sqrt{f2^2 - 4f1f3}$.

9.2. FUNCTIONS AND OPTIONS

Let us now describe the functions and options of the package in more detail and show how the user can apply them to concrete examples.

9.2.1. *RationalizeRoot*

When using the package for the first time, the **RationalizeRoot** function is an excellent way to get started. Without requiring any prior knowledge about the rationalization method, the user can provide a square root and obtain a variable change that turns this square root into a rational function. For example, consider the square root $\sqrt{1 - x^2 - y^2}$. To find a rationalizing change of variables, we can apply the package as follows:

```
RationalizeRoot [Sqrt[1-x^2-y^2]]
{{x → 2t[1] / (1+t[1]^2+t[2]^2), y → - (1-t[1]^2+t[2]^2) / (1+t[1]^2+t[2]^2)}}
```

With this substitution, we have $\sqrt{1 - x^2 - y^2} = 2t_1 t_2 / (t_1^2 + t_2^2 + 1)$.

Although **RationalizeRoot** is already quite powerful, it is considered a preliminary function. For example, **RationalizeRoot** will not rationalize nested square roots. Using **ParametrizePolynomial** instead, the user has more control over the hypersurface associated to the square root, which also allows for the rationalization of more general algebraic functions. Advanced users should, therefore, work with the **ParametrizePolynomial** function.

9.2.2. *ParametrizePolynomial*

As a first step, we demonstrate the basic usage of **ParametrizePolynomial** using the square root $\sqrt{1 - x^2 - y^2}$. Instead of the actual square root, we have to provide the defining polynomial of the associated hypersurface as input for the function:

```
ParametrizePolynomial[r^2+x^2+y^2-1]
{{r → 2t[1]t[2] / (1+t[1]^2+t[2]^2), x → 2t[1] / (1+t[1]^2+t[2]^2), y → - (1-t[1]^2+t[2]^2) / (1+t[1]^2+t[2]^2)}}
```

We see that, in addition to the change of variables, the output also contains the expression of the rationalized square root up to sign. Now that we understand the basic usage of **ParametrizePolynomial**, let us go through the different options of the function.

Variables

By default, **ParametrizePolynomial** performs the transformation in all variables of the input. Depending on the context, however, it can be advantageous to transform only a subset of the variables. The **Variables** option allows the user to specify which variables should be changed. For example, consider the rationalization of $\sqrt{x + y + 1}$. On the one hand, we can rationalize using:

```
ParametrizePolynomial[r^2-x-y-1]
{{r → 1+t[1] / t[2], x → 1+t[1] / t[2]^2, y → - (t[1]^2-t[1]+t[2]^2) / t[2]^2}}
```

On the other hand, we can use the **Variables** option to only change variables in y :

```
ParametrizePolynomial[r^2-x-y-1,Variables→{r,y}]
{{r → (1+x)t[1], y → -1-x+t[1]^2+2xt[1]^2+x^2t[1]^2}}
```

As we will see later, this option is particularly powerful when it comes to the simultaneous rationalization of multiple square roots. We want to point out that, although the output obtained in this way is guaranteed to be rational in the new variables (in this case $t[1]$), one might encounter new square roots

that depend on the variables we viewed as parameters (in this case x). We will provide a more detailed discussion of such an example in the last section.

OutputVariables

By default, the new variables of a transformation are called $t[1], t[2], \dots$, as we have already seen. Using the option `OutputVariables`, however, the user can specify the names of the new variables to be, for instance, v and w :

```
ParametrizePolynomial[r^2+x^2+y^2-1, OutputVariables→{v,w}]
{r→2vw/(1+v^2+w^2), x→2v/(1+v^2+w^2), y→-(1-v^2+w^2)/(1+v^2+w^2)}
```

This option is convenient when we apply the function iteratively to rationalize multiple square roots simultaneously.

MultipleSolutions

Setting `MultipleSolutions` to `True` provides the user with multiple rational parametrizations. These parametrizations are obtained by applying the algorithm multiple times using all the different $(d-1)$ -points across all affine charts of the projective closure of the given hypersurface.

GeneralC

Some square roots have an associated hypersurface with infinitely many $(d-1)$ -points. Consider, for instance, the square root $\sqrt{1-x^2}$, which is associated to the unit circle. The unit circle is a hypersurface of degree 2. Therefore, a $(d-1)$ -point is given by any regular point. The rational parametrization that the algorithm produces is, however, not independent of the choice of the $(d-1)$ -point. In fact, what point we choose will have an impact on the coefficients that we get in our variable change. To see this, we take $(r_0, x_0) = (\sqrt{3}/2, 1/2)$ as our $(d-1)$ -point, instead of our usual choice $(r_0, x_0) = (-1, 0)$. This produces rational parametrizations of the unit circle like

$$\phi_r(t) = \frac{\sqrt{3}}{2} - \frac{\sqrt{3} + t}{t^2 + 1}, \quad \phi_x(t) = \frac{1}{2} - \frac{t(\sqrt{3} + t)}{t^2 + 1}.$$

The `GeneralC` option encodes how the parametrization depends on the choice of the $(d-1)$ -point—in case there are infinitely many of these points. More precisely, if the option is enabled, the output will depend on free parameters

$C[1]$, $C[2]$, etc. By substituting concrete values for these parameters, the user is effectively fixing a $(d - 1)$ -point, in retrospect, which allows the user to find a change of variables that is most suitable in the given context. Applying the **GeneralC** option to the unit circle, we get:

```
ParametrizePolynomial[r^2+x^2-1, GeneralC→True]
{{r→-c[2]-2c[1]t[1]+c[2]t[1]^2
c[1]-2c[2]t[1]+c[1]t[1]^2, x→-√c[1]^2-c[2]^2-√c[1]^2-c[2]^2t[1]^2
c[1]-2c[2]t[1]+c[1]t[1]^2}}
```

Notice that at least one of the free parameters has to be chosen different from zero. In most cases, an integer choice of coordinates will produce the parametrizations that are least cluttered. Therefore, whenever possible, the package chooses integer coordinates if the **GeneralC** option is not specified.

GeneralT

The **GeneralT** option skips step 5 of the rationalization algorithm and leaves it to the user to set one of the new variables t_i equal to one in retrospect. This has the advantage that one can spot what choice of $t_i = 1$ produces the variable change that is most suitable in the user's context. As an example, let us consider the hypersurface associated to $\sqrt{x^3 + x^2}$. Applying the **GeneralT** option, we obtain:

```
ParametrizePolynomial[r^2-x^3-x^2, GeneralT→True]
{{r→t[1](-t[0]+t[1])(t[0]+t[1])
t[0]^3, x→(-t[0]+t[1])(t[0]+t[1])
t[0]^2}}
```

From this output, we see that we can simplify the variable change—in the sense that we avoid rational expressions—by choosing $t[0]=1$ instead of $t[1]=1$. Without setting **GeneralT** to **True**, the package would make a choice automatically, which does not necessarily lead to the most suitable result.

ForceFDecomposition

Some square roots have the property that their associated hypersurface has a $(d - 1)$ -point and is, also, F -decomposable. Consider, for instance, the following square root:

$$\sqrt{(1 - x_1 - x_2 - x_3)^2 - 4x_1x_2x_3}.$$

The associated hypersurface has several $(d - 1)$ -points, so the package will easily find multiple parametrizations. In particular, it will not apply the F -decomposition theorem to generate the output. We observe, however, that the square root is F -decomposable. Thus, we can use the **ForceFDecomposition** option to force an application of the F -decomposition theorem. This will give us variable changes that are, in general, different from the ones we get when not specifying the option. In this way, we are able to produce even more variable changes for square roots of that type.

FPolynomials

Notice that, whenever we apply the F -decomposition theorem, we have a freedom in choosing $f_{\frac{d}{2}-1}$, $f_{\frac{d}{2}}$, and $f_{\frac{d}{2}+1}$. For the above square root, two appropriate choices would be:

1. $f_1 = 1$, $f_2 = 1 - x_1 - x_2 - x_3$, $f_3 = x_1x_2x_3$,
2. $f_1 = x_1$, $f_2 = 1 - x_1 - x_2 - x_3$, $f_3 = x_2x_3$.

Making different choices for the f_i 's will result in different parametrizations. Therefore, it can be useful to try different choices of the f_i 's to optimize the final variable transformation. The user can specify a particular choice as follows: if the input polynomial is of the form

$$f := r^2 - f_{\frac{d}{2}}^2 + 4f_{\frac{d}{2}-1}f_{\frac{d}{2}+1},$$

then the user has to provide the list

$$\left\{ f_{\frac{d}{2}-1}, f_{\frac{d}{2}}, f_{\frac{d}{2}+1} \right\}.$$

Notice that, in order to apply the F -decomposition with this particular choice of f_i 's, one has to set **ForceFDecomposition** to **True** in case $V = \mathbb{V}(f)$ has a $(d - 1)$ -point.

9.3. ON THE ROLE OF SQUARES

It is now the right time to come back to the role of perfect squares in a rationalization procedure. We have seen that, especially in the process of rationalizing

multiple square roots, one often encounters square roots whose arguments contain factors that are perfect squares. Recall that a rationalization of the square root without the perfect square factor already gives a rationalization of the square root that includes the perfect square factor. For instance, consider the square root $\sqrt{x^3 + x^2} = \sqrt{(x+1)x^2}$. Since one of the factors of the argument is already a perfect square, it suffices to find a suitable variable change for the simpler square root $\sqrt{x+1}$, e.g., $x = t^2 - 1$, in order to rationalize $\sqrt{x^3 + x^2}$.

From the above example, one might be tempted to think that leaving out perfect squares is always a good idea. This is, however, not always true. In fact, both cases can occur:

1. Leaving out a perfect square can make the rationalization procedure easier:

The reader is invited to check that the package does not find a rational parametrization of $V = \mathbb{V}(r^2x^2 - x^4 - x^4y - xy^2 - x^2y^2)$, which is associated to the square root

$$\sqrt{\frac{x^4 + x^4y + xy^2 + x^2y^2}{x^2}}.$$

If we, however, leave out the perfect square in the denominator and instead consider

$$\sqrt{x^4 + x^4y + xy^2 + x^2y^2}$$

with the associated hypersurface $W = \mathbb{V}(r^2 - x^4 - x^4y - xy^2 - x^2y^2)$, then the package will find a parametrization. This result can then, of course, also be used to rationalize the square root we wanted to rationalize in the first place.

2. Leaving out a perfect square can make the rationalization procedure harder:

Suppose we want to rationalize

$$\sqrt{\frac{x^4 + 4x^2y^2 + 4}{4x^2}}.$$

The reader can check that leaving out the perfect square in the denominator, i.e., considering

$$\sqrt{x^4 + 4x^2y^2 + 4},$$

leads to an associated hypersurface $V = \mathbb{V}(r^2 - x^4 - 4x^2y^2 - 4)$, which does not have a single $(d - 1)$ -point. The package will still find a rational parametrization, but only after employing the F -decomposition theorem.

If we, however, try to rationalize the original square root by considering $W = \mathbb{V}(4r^2x^2 - x^4 - 4x^2y^2 - 4)$, we have already seen that W has a $(d - 1)$ -point at infinity. Therefore, we can directly apply the algorithm so that, in this particular case, it is advantageous to keep the perfect square for the rationalization procedure.

From these two examples, we learn that it is a worthwhile exercise for the user to factor the perfect squares of the argument of the square root and try to find rationalizations while keeping and leaving out perfect squares as above. With this strategy, one can produce different, possibly refined variable transformations, which sometimes even will allow for the rationalization of square roots that were—on first sight—not rationalizable by our methods.

9.4. RATIONALIZATION VIA VARIABLES OPTION

The purpose of this final section is to illustrate the usefulness of the **Variables** option, which can be crucial in the simultaneous rationalization of multiple square roots. Suppose we want to rationalize

$$\{\sqrt{1 - x^2}, \sqrt{1 - x^2 - y^2}\}.$$

Starting with the rationalization of the second square root, we find:

```
ParametrizePolynomial[r[1]^2+x^2+y^2-1,OutputVariables→{v,w}]
{{r[1]→2vw/(1+v^2+w^2),x→2v/(1+v^2+w^2),y→2w^2/(1+v^2+w^2)-1}}
```

The next step is to substitute the above expression for x into $\sqrt{1-x^2}$ and try to rationalize the resulting square root. We observe, however, that the package is not able to find a rationalization:

```
ParametrizePolynomial[r[2]^2(1+v^2+w^2)^2+4v^2-(1+v^2+w^2)^2]
{}
```

In such a case, the user might be tempted to think that the given set of square roots cannot be rationalized with the package. There is, however, a way in which we can still succeed, namely by using the **Variables** option. We start again by rationalizing $\sqrt{1-x^2-y^2}$, but this time we specify the **Variables** option as follows:

```
ParametrizePolynomial[r[1]^2+x^2+y^2-1,Variables→{r[1],y},
OutputVariables→{w}]
{{r[1]→2w(x^2-1)/(x^2-1)w^2-1,y→(sqrt(1-x^2)((x^2-1)w^2+1))/(x^2-1)w^2-1}}
```

We see that the transformation is rational in the new variable w , but contains a square root in the variable x that we did not specify to be a variable of the input polynomial. This square root in x is, however, the second square root of our original set. Because the rationalization of $\sqrt{1-x^2-y^2}$ happened only via a change in y , the other original square root $\sqrt{1-x^2}$ does not change under this transformation. Thus, we can rationalize the remaining square root via $x = (v^2 - 1)/(v^2 + 1)$, as discussed previously. Substituting this expression for x in the transformation of y yields:

$$x = \frac{v^2 - 1}{v^2 + 1}, \quad y = -\frac{2v(1 + v^4 + v^2(2 - 4w^2))}{(1 + v^2)(1 + v^4 + v^2(2 + 4w^2))}.$$

Indeed, we can check that these substitutions turn the initial square roots into rational functions of v and w :

$$\sqrt{1-x^2} = \frac{2v}{v^2 + 1}, \quad \sqrt{1-x^2-y^2} = \frac{8v^2w}{1 + v^4 + v^2(2 + 4w^2)}.$$

Conclusions and Outlook

In this thesis, we studied the question of how to rationalize sets of square roots that appear in the computation of Feynman integrals. We addressed the problem by relating it to one of the most fundamental questions in algebraic geometry, namely the rationality problem for hypersurfaces.

On the one hand, we have seen that not all square roots are rationalizable. We used several known results from the theory of curves and surfaces to establish rigorous criteria for the non-rationalizability of a given set of square roots. We clarified these techniques through examples of physical relevance.

On the other hand, we discussed an algorithm that yields a rationalization of a given square root whenever the associated hypersurface has a point of multiplicity $d - 1$, where d is the degree of the hypersurface. This algorithm covers many cases from high energy physics that admit a rational parametrization. In addition, we presented the F -decomposition theorem, which enables the rationalization of many square roots that would otherwise not be rationalizable by our methods.

Furthermore, we presented the `RationalizeRoots` software package that implements our rationalization techniques in **Mathematica**. A detailed account on the **Maple** version of the package can be found in [1].

The results of this thesis are broadly applicable in many Feynman integral computations. For physics applications of the last two years, where the presented techniques were of relevance, we refer the reader to [13]–[16], [87]–[103].

Finally, let us give some suggestions for future work: one possible future project would be a further refinement of our non-rationalizability criteria. In this thesis,

we mainly focused on the case of curves and double coverings of the projective plane. One could, for example, collect special cases of hypersurfaces beyond two dimensions that are associated to a square root and known to be not parametrizable by rational functions.

There may also be several ways to expand the current version of our rationalization algorithm. For example, one might be able to formulate other theorems like the F -decomposition theorem that would allow to use parametrization by lines for hypersurfaces that do not have a $(d - 1)$ -point. Furthermore, there are some univariate square roots that `RationalizeRoots` will not be able to rationalize. Although none of these cases is known to be of physical relevance, for the sake of completeness, it would be good to add the parametrization by adjoints technique [23] to the package. This would enable our software to rationalize *all* rationalizable univariate square roots.

Finally, there is a **Singular** library, called `classify2.lib`, which can be used to classify simple curve singularities. While we focused on **Magma** in this thesis, it would be beneficial for the physics community to explain how to classify singularities with this free, open source alternative.

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08/2007–06/2010 **Gymnasium Taunusstein**
Degree: Allgemeine Hochschulreife

Work Experience

05/2017–03/2020 **Research Associate, University of Mainz**
Research and Academic Teaching in Mathematics and Physics

05/2017–10/2018 **Trainee, d-fine GmbH**
Full Stack Web Application Development

02/2017–04/2017 **Intern, d-fine GmbH**
Front End Web Application Development

04/2012–06/2016 **Research Assistant, University of Mainz**
Academic Teaching in Mathematics and Physics

Further Skills

Languages: German (Native Tongue)
English (Fluent)
Russian (Basics)
Latin (Basics)

Nanodegree: Udacity Nanodegree “AI Programming with Python”

IT: Python, PyTorch, Git, Oracle Stack

List of Publications

- 1 M. Besier, D. van Straten, and S. Weinzierl, “Rationalizing roots: an algorithmic approach”, *Communications in Number Theory and Physics*, vol. 13, 2019. arXiv: [1809.10983](https://arxiv.org/abs/1809.10983).
- 2 M. Besier, D. Festi, M. Harrison, and B. Naskrecki, “Arithmetic and geometry of a K3 surface emerging from virtual corrections to Drell–Yan scattering”, 2019. arXiv: [1908.01079](https://arxiv.org/abs/1908.01079).
- 3 M. Besier, P. Wasser, and S. Weinzierl, “RationalizeRoots: Software Package for the Rationalization of Square Roots”, 2019. arXiv: [1910.13251](https://arxiv.org/abs/1910.13251).