Supersymmetric Quantum Mechanics with periodic potentials

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Abstract

The formalism of supersymmetric quantum mechanics is discussed, and used to analyze a particle in one-dimensional, non-relativistic conditions travelling under the influence of a potential constructed from the superpotential $\sigma = \ell \cdot m\frac{\mathrm{sn}(x,m)\mathrm{cn}(x,m)}{\mathrm{dn}(x,m)}$. This superpotential is of special interest, since it gives rise to a class of so called associated Lamé potentials, semi-analytically solvable periodic potentials that represent a generalization of the Lamé potentials. First, the non-periodic case ($m = 1$) is considered, especially regarding its scattering properties. Ultimately, the periodic case ($m \neq 1$) is studied giving special attention to the band gaps in the spectrum of the potential. A numerical approach will also be presented based upon the Floquet-Lyapunov theory, and the Lamé potentials will be qualitatively discussed using this approach. The features of the elliptic functions will be presented in the Appendix.

Acknowledgements

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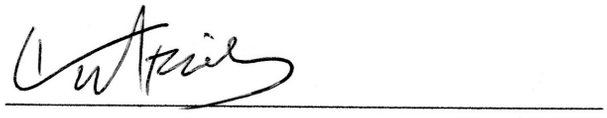
This Thesis is dedicated to my grandfather, who passed on to me the importance of discipline and order for success in difficult endeavours.

Statement

I hereby declare, that this thesis is my original work and was made using only the cited sources. I also state, that all citations have been properly acknowledged and that this thesis was not used in any form to meet past examination requirements nor was it published as a scientific paper.



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CHAPTER 1

Motivation

The set of analytically solvable problems in physics, and particularly in quantum mechanics, represents a very small subset of all interesting physical problems. This may be rooted in the fact that, in most cases, a symmetry of some kind must be present in the setting of it, in order to be analytically solvable. For this reason, any formalism that allows to enlarge this small set connotes an important leap in the understanding of the field, for it may shed a light upon a newly discovered symmetry. Supersymmetric quantum mechanics (SUSY QM) is such a formalism, and it creates a symmetry by factorizing the Hamiltonian into selfadjoint operators (usually two). As will soon be shown, this factorization will allow to link degenerate eigenvalues of the Hamiltonian and therefore reduce the problem significantly. In fact, this formalism is able to produce exact results elegantly.

The core idea of supersymmetry resides in quantum field theory as an attempt to explain a mysterious asymmetry between gauge fields and matter fields; the former being bosonic and the latter fermionic. For this it was proposed in the second half of the 20^{th} century to unite the internal and external symmetries of a system by introducing so-called supersymmetric partners to each observed particle with contrasting fermionic or bosonic nature, as the case may be. To further illustrate this relation see fig. 1.1. A more thorough explanation of this topic may be found in [Wei05].

Because this formalism is able to provide exact results, it can be a useful tool in analyzing periodic potentials. Even in one dimension, periodic potentials are used widely in solid sate physics to model the crystalline structure of materials, which can in turn provide important information about their electronic properties.

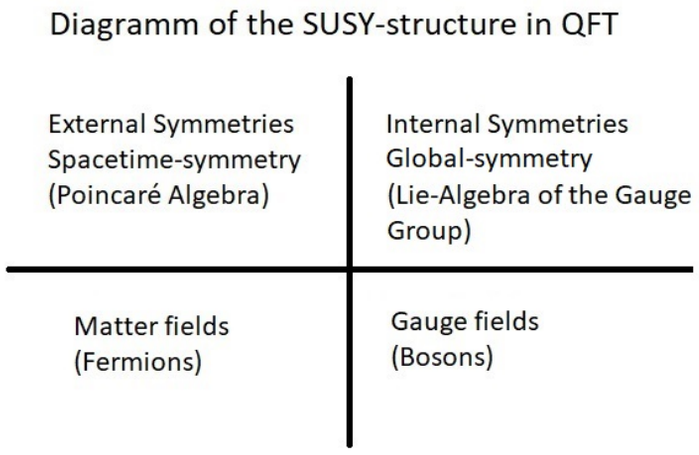

FIGURE 1.1: Table illustrating relation between fermions and bosons in supersymetric quantum field theory. The goal of SUSY is to unify the spacetime-symmetry with the global symmetry. This implies a unification of sorts of the fermions with the bosons.

To illustrate the typical behaviour of a periodic potential, consider for example a one dimensional well-potential. The bound states are solutions of the Schrödinger equation with proper boundary conditions. For two well-potentials sufficiently far apart from each other, the bound states do not interact. This only leads to a degeneration of the bound-state-energies, since each potential harbours independently the same eigenstates. Do, however, the bound states of the potentials interact with each other, so is each energy level split in two. When considering an array of infinitely many well potentials interacting with one-another, the energy values are forced to become energy-bands, and the eigenfunctions are subjected to the Bloch condition. The topic of exact solvable periodic potentials is discussed in [KS04].

CHAPTER 2

Formalism of Supersymmetric Quantum Mechanics

Symmetries play a very important role in any field of physics. In physics it is said, that a given system has a symmetry if any of its describing properties is left invariant under certain transformations. Mathematically, this can be described with the help of a group, whose form will depend on the kind of symmetry that is being explored. In the case of supersymmetry, the unification of the external and internal symmetries is the goal, which implies a unification of the Poincaré- and the Lie-algebra of the gauge group that describe them respectively (see fig. 1.1). A general form of this unification will be discussed in the following section, whereas a special case is to be explored in the subsequent section.

2.1 General Formalism

Even though a deep discussion of the concept of Lie-groups and Lie-algebras lies beyond the scope of this consideration, a small definition may not be out of order. A deeper discussion of this topic, regarding physical systems may be found in [Wip06].
The Lie-algebra of a Lie-group is a vector space with a bilinear mapping tangent to the identity element of the group, that is anti-symmetric, and satisfies the Jacobi identity. In physics, the mapping is often taken as the usual commutator of quantum mechanics defined as

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad . \tag{2.1}$$

However, in order to unify the aforementioned algebras (in a non-trivial manner) it is necessary to expand the Lie-algebra by introducing another mapping, characterized with the same

properties of the usual anti-commutator

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A} \quad . \tag{2.2}$$

A Lie-algebra with these properties is known as a superalgebra.
[Jun12] defines a supersymmetric quantum-mechanical system by introducing the superalgerbra to a usual quantum system. Consider a quantum system characterized by a Hamiltonian $\hat{\mathscr{H}}$ acting on a (rigged) Hilbert-space $\mathcal{H}$ (see [Mad05]). Let $\hat{Q}_i = \hat{Q}_i^{\dagger}$ (with $i = 1, \ldots, N$) be N self-adjoint operators acting on $\mathcal{H}$.

DEFINITION 1. *A quantum system characterized by the set $\{\hat{\mathscr{H}}, \hat{Q}_1, \ldots, \hat{Q}_N; \mathcal{H}\}$ is supersymmetric if for all $i, j = 1, \ldots, N$*

$$\{\hat{Q}_i, \hat{Q}_j\} = \hat{\mathscr{H}}\delta_{ij}\,, \tag{2.3}$$

The $\hat{Q}_i$´s are called supercharges, the corresponding symmetry is called N-extended supersymmetry and $\hat{\mathscr{H}}$ is called a supersymmetric Hamiltonian.

Therefore, the SUSY-Hamiltonian is given by

$$\hat{\mathscr{H}} = 2\hat{Q}_1^2 = 2\hat{Q}_2^2 = \cdots = \frac{2}{N}\sum_{i=1}^{N}\hat{Q}_i^2 \quad , \tag{2.4}$$

which, in turn implies for all $i \in \{1, 2, \ldots, N\}$

$$[\hat{\mathscr{H}}, \hat{Q}_i] = 0 \quad , \tag{2.5}$$

since $\hat{\mathscr{H}}$ is an analytic function of a given supercharge. Therefore, the supercharges are constants of motion if they do not depend explicitly on time.
Due to the spectral theorem, the quadratic structure of the SUSY Hamiltonian (see eq. 2.4), and the fact that the $\hat{Q}_i$´s are self-adjoint, it follows that the spectrum of the Hamiltonian is non-negative

$$spec(\hat{\mathscr{H}}) \subseteq \mathbb{R}^{+} \quad . \tag{2.6}$$

This applies in particular to the ground energy level $E_0 := \inf(spec(\hat{\mathscr{H}}))$, which is the decisive factor to consider, when describing if the supersymmetry of a system is *broken* or *unbroken*. These concepts are defined below.

DEFINITION 2. *A super-symmetric quantum mechanical system has an unbroken (good or exact) supersymmetry if $E_0 = 0$. Conversely, for $E_0 > 0$ the supersymmetry is broken*

2.2 The Case of a $N = 2$ Extended Supersymmetry

The most widely used, and discussed case of SUSY QM, and indeed the one used in the following chapters, is the case of $N = 2$ extended supersymmetry. For this case (and for $N > 2$) the aforementioned construction allows for a supersymmetric transformation that links degenerate Eigenvalues of the supersymmetric Hamiltonian $\hat{\mathscr{H}}$.

2.2.1 Complex Supercharges

Setting $N = 2$ implies in first line regarding definition 1

$$\{\hat{Q}_1, \hat{Q}_2\} = 0 \iff \hat{Q}_1\hat{Q}_2 = -\hat{Q}_2\hat{Q}_1 \tag{2.7}$$

and

$$\hat{\mathscr{H}} = 2\hat{Q}_1^2 = 2\hat{Q}_2^2 = \hat{Q}_1^2 + \hat{Q}_2^2 \quad . \tag{2.8}$$

For convenience, we may introduce the so-called complex supercharges $\hat{Q}$ and $\hat{Q}^\dagger$ given by

$$\hat{Q} := \frac{1}{\sqrt{2}}(\hat{Q}_1 + i\hat{Q}_2) \tag{2.9}$$

and

$$\hat{Q}^\dagger := \frac{1}{\sqrt{2}}(\hat{Q}_1 - i\hat{Q}_2) \tag{2.10}$$

which, satisfy

$$\hat{Q}^2 = 0 = \hat{Q}^{\dagger 2}, \quad \text{and} \quad \{\hat{Q}, \hat{Q}^\dagger\} = \hat{\mathscr{H}} \quad . \tag{2.11}$$

Many authors restrict their definition of a supersymmetric system to this algebra for $N = 2$ because this is the case originally discussed in the genesis of supersymmetric quantum

mechanics.

Equation 2.11 allows the complex supercharges to be represented by nilpotent matrices

$$\hat{Q} = \begin{pmatrix} 0 & 0 \\ \hat{A} & 0 \end{pmatrix} \quad \hat{Q}^\dagger = \begin{pmatrix} 0 & \hat{A}^\dagger \\ 0 & 0 \end{pmatrix} \quad , \tag{2.12}$$

for some operator $\hat{A}$. Before exploring the properties of this operator, consider the representation of $\hat{\mathscr{H}}$ that is implied hereby,

$$\hat{\mathscr{H}} = \{\hat{Q}, \hat{Q}^\dagger\} = \begin{pmatrix} \hat{A}^\dagger\hat{A} & 0 \\ 0 & \hat{A}\hat{A}^\dagger \end{pmatrix} := \begin{pmatrix} \hat{\mathscr{H}}^- & 0 \\ 0 & \hat{\mathscr{H}}^+ \end{pmatrix} \quad , \tag{2.13}$$

and notice that due to the diagonal nature of the representation, the SUSY Hamiltonian may be decomposed into two so-called supersymmetric partner Hamiltonians $\hat{\mathscr{H}}^\pm$. Notice, that the partner Hamiltonians are self-adjoint, and thus their spectrum is well-defined. Since the Hilbert-space is rigged, the considered states may be elements of the spaces of linear and antilinear functionals, which allows for both the usual square integrable functions, as well as for the so called distributions to describe states. This allows for a more rigorous approach to improper (or scattering) eigenstates, characterized by a distribution and an associated continuous spectrum, as well as to normalizable bound states. The rigged Hilbert-space is often characterized as a usual Hilbert-space equipped with distribution theory.

Let

$$\hat{\mathscr{H}}^\pm|\psi_n^\pm\rangle = E_n^\pm|\psi_n^\pm\rangle \tag{2.14}$$

be the eigenvalue equation for the partner Hamiltonians. Then, according to eq. 2.12, any given eigenstate of $\hat{\mathscr{H}}$ is either given by

$$|\psi_n\rangle = \begin{pmatrix} |\psi_n^-\rangle \\ 0 \end{pmatrix} \quad \text{or} \quad |\psi_n\rangle = \begin{pmatrix} 0 \\ |\psi_n^+\rangle \end{pmatrix} \quad . \tag{2.15}$$

This implies,

$$\hat{\mathscr{H}} \begin{pmatrix} |\psi_n^-\rangle \\ 0 \end{pmatrix} = E_n^- \begin{pmatrix} |\psi_n^-\rangle \\ 0 \end{pmatrix} \quad |\hat{Q}\cdot$$

$$\Leftrightarrow \hat{Q}\hat{\mathscr{H}} \begin{pmatrix} |\psi_n^-\rangle \\ 0 \end{pmatrix} = \hat{Q}E_n^- \begin{pmatrix} |\psi_n^-\rangle \\ 0 \end{pmatrix}$$

$$\xRightarrow[\text{see 2.4}]{[\hat{\mathscr{H}},\hat{Q}_i]=0} \hat{\mathscr{H}}\hat{Q} \begin{pmatrix} |\psi_n^-\rangle \\ 0 \end{pmatrix} = E_n^-\hat{Q} \begin{pmatrix} |\psi_n^-\rangle \\ 0 \end{pmatrix} \quad ,$$

and hence,

$$\hat{Q} \begin{pmatrix} |\psi_n^-\rangle \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \hat{A}|\psi_n^-\rangle \end{pmatrix} \tag{2.16}$$

is an eigenstate of the SUSY Hamiltonian. This relation allows for the discussion of $\hat{A}$ to be properly made.

2.2.2 Annihilation and Creation Operators

In order to discuss the significance of $\hat{A}$, consider equations 2.13 and 2.16 in its capacity of eigenstate of the SUSY Hamiltonian. Together this implies

$$\hat{\mathscr{H}}^+(\hat{A}|\psi_n^-\rangle) = E_n^-(\hat{A}|\psi_n^-\rangle) \quad . \tag{2.17}$$

Analogously, it follows for $\hat{\mathscr{H}}^-$

$$\hat{\mathscr{H}}^-(\hat{A}^\dagger|\psi_n^+\rangle) = E_n^+(\hat{A}^\dagger|\psi_n^+\rangle) \quad . \tag{2.18}$$

This result links therefore the partner Hamiltonians via $\hat{A}$, assuming the energy-levels to be greater than zero. The case of a vanishing energy level corresponds to the ground level of an unbroken SUSY system. A general consideration of such a system can be done, to further explore the repercussions in a 2-extended supersymmetric case.

PROPOSITION 1. *Let $|\psi_0\rangle$ be the normalized ground state of a super-symmetric Hamiltonian. Then, for an unbroken super-symmetry, any supercharge acting upon the ground state yields*

the zero eigenvector,

$$E_0 = 0 \Leftrightarrow \forall i : \hat{Q}_i|\psi_0\rangle = 0\,. \tag{2.19}$$

Conversely, for a broken super-symmetry, it is always possible to find a supercharge, for which acting on the ground state yields a non-zero vector,

$$E_0 > 0 \Leftrightarrow \exists i : \hat{Q}_i|\psi_0\rangle \neq 0\,. \tag{2.20}$$

A similar statement can be done for an orthonormal system of the ground eigenspace.

PROOF. The statement of eq.2.20 is only the logic negation of eq.2.19, provided all values of E_0 are not negative, which is the case, according to eq.2.6. Hence it suffices to consider only the case where the ground energy disappears:
it holds for the ground energy

$$\hat{\mathscr{H}}|\psi_0\rangle = E_0|\psi_0\rangle\,, \tag{2.21}$$

and eq.2.4 implies

$$\frac{2}{N}\sum_{i=1}^{N}\hat{Q}_i^2|\psi_0\rangle = E_0|\psi_0\rangle \quad . \tag{2.22}$$

Further, the supercharges are self-adjoint and hence

$$\sum_{i=1}^{N}\langle\psi_0|\hat{Q}_i^\dagger\hat{Q}_i|\psi_0\rangle = \frac{E_0 N}{2}\,. \tag{2.23}$$

This equation yields for $E_0 = 0$, and for all i

$$\|\hat{Q}_i|\psi_0\rangle\|^2 = 0 \tag{2.24}$$

which evidently proofs the proposition.

□

For the case of $N = 2$ with the aforementioned representation, the ground state of the SUSY Hamiltonian is either

$$|\psi_0\rangle = \begin{pmatrix} |\psi_0^-\rangle \\ 0 \end{pmatrix} \quad \text{or} \quad |\psi_0\rangle = \begin{pmatrix} 0 \\ |\psi_0^+\rangle \end{pmatrix} \quad . \tag{2.25}$$

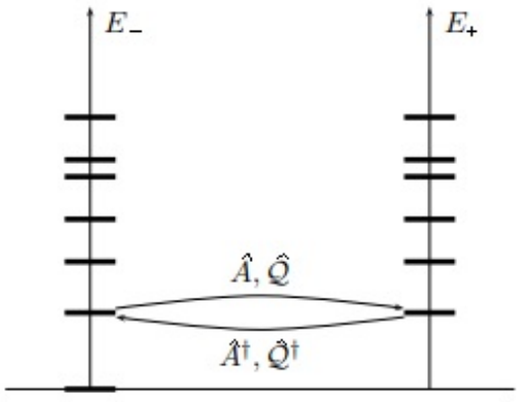

FIGURE 2.1: Diagram showing schematically the link between the spectra of two partner Hamiltonians. Adapted from [Wip00].

Because of this, the proposition 1, and the structure of the complex supercharges it follows,

$$\hat{A}|\psi_0^-\rangle = 0 \quad \text{or} \quad \hat{A}^\dagger|\psi_0^+\rangle = 0 \quad , \tag{2.26}$$

and thus $|\psi_0^\pm\rangle$ are not paired with another eigenstate as shown in equations 2.17 and 2.18. These relations lead to the following definition,

$$|\psi_n^+\rangle := \frac{1}{\sqrt{E_{n+1}^-}}\hat{A}|\psi_{n+1}^-\rangle \quad \text{and} \quad |\psi_n^-\rangle := \frac{1}{\sqrt{E_{n-1}^+}}\hat{A}^\dagger|\psi_{n-1}^+\rangle \quad . \tag{2.27}$$

Therefore, $\hat{A}$ denotes an annihilation and $\hat{A}^\dagger$ a creation operator, as can be seen in fig. 2.1. Further, the corresponding eigenvalue equations yield $E_{n-1}^+ = E_n^-$. This behaviour is known as isospectrality between the partner Hamiltonians. It is important to remark, that for a finite spectrum of the Hamiltonian $\hat{\mathscr{H}}$, the spectra of the partner Hamiltonians will differ both in the ground state and in the state with eigenvalue $E_{max} := \max(spec(\hat{\mathscr{H}}))$.

2.2.3 Superpotential

For convenience, the units will be chosen such that, $\hbar = 1 = 2m$. In this section, partner Hamiltonians of the form

$$\hat{\mathscr{H}}^{\pm} = \hat{p}^2 + V^{\pm}(\hat{x}) = -\frac{d^2}{dx^2} + V^{\pm}(x) \quad , \tag{2.28}$$

considered in [GMR17], will be analyzed in order to develop a more specialized formalism. Since the potential characterizes this type of Hamiltonian, it is helpful to decompose $\hat{A}$ in such a way, that allows the potential to be discussed independently. A standard way of doing this is by defining

$$\hat{A} := i\hat{p} + \sigma(\hat{x}) = \frac{d}{dx} + \sigma(x) \quad \text{and thus} \quad \hat{A}^{\dagger} = -\frac{d}{dx} + \sigma(x) \quad . \tag{2.29}$$

σ denotes the so-called superpotential, which gives rise to the standard potential via 2.13 and the canonical conmutation relation $[\hat{x}, \hat{p}] = \mathbb{1}i$. Together they yield the partner Hamiltonians

$$\begin{aligned} \hat{\mathscr{H}}^{+} &= \hat{A}\hat{A}^{\dagger} = -\frac{d^2}{dx^2} + \sigma^2(x) + \frac{d\sigma(x)}{dx} \quad , \\ \text{and} \quad \hat{\mathscr{H}}^{-} &= \hat{A}^{\dagger}\hat{A} = -\frac{d^2}{dx^2} + \sigma^2(x) - \frac{d\sigma(x)}{dx} \quad . \end{aligned} \tag{2.30}$$

And hence the potential is given by

$$V^{\pm}(x) = \sigma^2(x) \pm \frac{d\sigma(x)}{dx} \quad . \tag{2.31}$$

Consider the implication of this definition on the ground state of an unbroken SUSY-system. Plugging in eq. 2.29 in eq.2.26, yields a first order ordinary differential equation,

$$\hat{A}|\psi_0^-\rangle = \left(\frac{d}{dx} + \sigma(x)\right)\psi_0^-(x) = 0 \quad . \tag{2.32}$$

For a given superpotential, this ODE may be used to find the ground state of the system

$$\psi_0^-(x) = Me^{-\int_{-\infty}^{\infty}\sigma(x)dx} \quad , \tag{2.33}$$

With M a normalizing constant. Analogously, this process could be undertaken for the ODE corresponding to $\hat{A}^{\dagger}$. This ODE yields

$$\psi_0^+(x) = \tilde{M} e^{+\int_{-\infty}^{\infty} \sigma(x) dx} \quad . \tag{2.34}$$

Notice that if in one case the exponential remains bounded, then it must grow without boundary in the other case. Thus at most one of the partner Hamiltonians has a vanishing ground energy, and at most one of the equations above will be meaningful for a given system.

CHAPTER 3

Non-periodic Case

It may be helpful to start the consideration of the superpotential $\sigma = \ell \cdot m\frac{\mathrm{sn}(x,m)\mathrm{cn}(x,m)}{\mathrm{dn}(x,m)}$ that belongs to the associated Lamé potentials, by considering the hyperbolic limit of the elliptic functions. The parameter m may be compared to the eccentricity of an ellipse centered at the origin, with semi-major and -minor axes aligned with the x- and y- axis respectively and with a normalized semi-minor axis. For this reason $m = 0$ corresponds to a perfect circle, and $m = 1$ approaches a hyperbola. The case of $m = 0$ is rather trivial, since the superpotential vanishes and the problem simply becomes a free particle problem. For $m = 1$, the aforementioned superpotential can be written as $\sigma = \ell \tanh(x)$ which gives rise to a non-trivial non-periodic potential. This extreme case will be handled in this chapter.

3.1 Spectrum of the Hyperbolic System

Using the techniques discussed in chapter 2, and based on [Jaf09] it is possible to find an elegant algebraic solution to the potential arising from $\sigma(x)$.
Since the superpotential is given, the lowering and rising operators can be immediately found using eq. 2.29.

$$\hat{A} = i\hat{p} + \ell \tanh(\hat{x}) \quad , \quad \hat{A}^\dagger = -i\hat{p} + \ell \tanh(\hat{x}) \quad . \tag{3.1}$$

Using the canonical commutation relation $[\hat{x}, \hat{p}] = \mathbb{1}i$ the supersymmetric partner Hamiltonians yield

$$\hat{\mathscr{H}}_\ell^+ = \hat{A}\hat{A}^\dagger = \hat{p}^2 - \ell(\ell-1)\mathrm{sech}(\hat{x})^2 + \ell^2 \quad , \tag{3.2}$$

and

$$\hat{\mathscr{H}}_\ell^- = \hat{A}^\dagger \hat{A} = \hat{p}^2 - \ell(\ell+1)\mathrm{sech}(\hat{x})^2 + \ell^2 \quad . \tag{3.3}$$

Notice that when ℓ differs by 1, both Hamiltonians only differ by a constant (2ℓ-1). This allows to link them simply by

$$\hat{\mathscr{H}}_\ell^+ = \hat{\mathscr{H}}_{\ell-1}^- + 2\ell - 1 \quad , \tag{3.4}$$

which in turn implies that the partner Hamiltonians have the same spectrum, only differing by a constant shift.

Eq. 2.32 yields a differential equation for the ground states dependent on ℓ for an unbroken SUSY, assuming $\hat{\mathscr{H}}_\ell^-$ to be the partner Hamiltonian with the ground energy,

$$(\partial_x + \ell \tanh(x))\psi_{0,\ell}^-(x) = 0 \quad , \tag{3.5}$$

the solution of which is

$$\psi_{0,\ell}^-(x) = M\mathrm{sech}(x)^\ell \quad . \tag{3.6}$$

With M an undetermined normalization constant.

Further, it is possible to find a connection of the spectra of $\hat{\mathscr{H}}_\ell^-$ depending on ℓ. Consider the following construction, with $|\psi_{\ell+1}^-\rangle$ an eigenstate of $\hat{\mathscr{H}}_{\ell+1}^-$ belonging to the eigenvalue $E_{\ell+1}^- > 0$.

$$\begin{aligned}
\hat{\mathscr{H}}_{\ell+1}^-|\psi_{\ell+1}^-\rangle &= E_{\ell+1}^-|\psi_{\ell+1}^-\rangle \quad |\hat{A}_{\ell+1}\cdot \\
\hat{A}_{\ell+1}\hat{A}^\dagger{}_{\ell+1}\hat{A}_{\ell+1}|\psi_{\ell+1}^-\rangle &= E_{\ell+1}^-\hat{A}_{\ell+1}|\psi_{\ell+1}^-\rangle \\
\hat{\mathscr{H}}_{\ell+1}^+\hat{A}_{\ell+1}|\psi_{\ell+1}^-\rangle &= E_{\ell+1}^-\hat{A}_{\ell+1}|\psi_{\ell+1}^-\rangle \\
(\hat{\mathscr{H}}_\ell^- + 2\ell + 1)\hat{A}_{\ell+1}|\psi_{\ell+1}^-\rangle &= E_{\ell+1}^-\hat{A}_{\ell+1}|\psi_{\ell+1}^-\rangle \\
\hat{\mathscr{H}}_\ell^-\hat{A}_{\ell+1}|\psi_{\ell+1}^-\rangle &= (E_{\ell+1}^- - 2\ell - 1)\hat{A}_{\ell+1}|\psi_{\ell+1}^-\rangle.
\end{aligned} \tag{3.7}$$

This makes clear that $\hat{\mathscr{H}}_\ell^-$ and $\hat{\mathscr{H}}_{\ell+1}^-$ have the same eigenstates without considering the ground state. Going from ℓ to $\ell+1$ shifts all eigenstates up by a constant and allows a new ground state at the bottom. Since for $\ell = 0$ the Hamiltonian describes a free particle, the Hamiltonians for all ℓ have a continuous spectrum above some energy level.
Further, this implies

$$\hat{A}_{\ell+1}|\psi_{\ell+1}^-\rangle \sim |\psi_\ell^-\rangle \Rightarrow \hat{\mathscr{H}}_{\ell+1}^-|\psi_{\ell+1}^-\rangle \sim E_{\ell+1}^-|\psi_{\ell+1}^-\rangle \sim \hat{A}_{\ell+1}^\dagger|\psi_\ell^-\rangle \quad , \tag{3.8}$$

which allows to construct new eigenstates with old ones, and will prove to be the key relation in solving this potential algebraically.

3.1.1 $\ell = 0$

Since the form of the partner potentials only differ by a constant shift, it suffices to solve only one of them. In order to keep the assumption above, and remain in the case of unbroken SUSY, consider $\hat{\mathscr{H}}_\ell^-$. For $\ell = 0$ this yields a free particle problem, for which an orthogonal system of eigenstates $|k_0^{\leftrightarrows}\rangle$ is known

$$\psi_0^{\leftrightarrows}(x,k) := \langle x|k_0^{\leftrightarrows}\rangle = \frac{1}{\sqrt{2\pi}} e^{\mp ikx} \quad , \tag{3.9}$$

where the square root normalizes the functions to a Dirac delta distribution. Nevertheless, eq. 2.26 applies and yields a constant ground state for this system. Notice that, in this context, ψ_0 does not denote the ground state anymore. It denotes instead the scattering state of $\ell = 0$.

3.1.2 $\ell = 1$

For $\ell = 1$ it suffices to compute the ground state (the only bound state) and the continuous states. The former can be done using equation 3.6 and the latter may be computed using the outcome of eq. 3.8 for the scattering state $|k_{\ell-1}\rangle$

$$\hat{A}_\ell^+|k_{\ell-1}\rangle \sim |k_\ell\rangle \quad . \tag{3.10}$$

Applying this to $\ell = 1$ and using eq. 3.9 yields

$$\langle x|\hat{A}_1^\dagger|k_0^{\leftrightarrows}\rangle \sim \psi_1^{\leftrightarrows}(x,k) \sim (-\frac{\partial}{\partial x} + \tanh(x))\frac{e^{\mp ikx}}{\sqrt{2\pi}} = (-ik + \tanh(x))\frac{e^{\mp ikx}}{\sqrt{2\pi}} \quad . \quad (3.11)$$

This state however, is not properly normalized, because the transmission and reflection due to the potential is not being considered. In the following section, this interaction is explored in order to find a normalization of these scattering states.

3.1.2.1 Scattering Properties

In order to properly normalize the scattering states, it is necessary to consider both the Reflection and Transmission coefficients (R and T resp.). These coefficients characterize the properties of a wave-function, which scatters with a given potential hindrance. They may be defined via the properties they ought to have for large x-values,

$$\sqrt{2\pi}\lim_{x\to\infty}\psi_{\rightarrow}(x) = T(k)e^{ikx} \quad , \quad \sqrt{2\pi}\lim_{x\to-\infty}\psi_{\rightarrow}(x) = e^{ikx} + R(k)e^{-ikx} \quad . \quad (3.12)$$

Notice, that the definition given above for T and R applies for a right travelling wave function. The left travelling wave can be easily defined by considering the properties of such a state for large x-values, namely by,

$$\sqrt{2\pi}\lim_{x\to\infty}\psi_{\leftarrow}(x) = e^{-ikx} + \bar{R}(k)e^{ikx} \quad , \quad \sqrt{2\pi}\lim_{x\to-\infty}\psi_{\leftarrow}(x) = \bar{T}(k)e^{-ikx} \quad , \quad (3.13)$$

where the bar on the coefficients highlights the fact, that they must not correspond to the coefficients of the right travelling wave.

After applying the parametrization for scattering states with the help of the transmission and reflection coefficients, $\psi_1^{\rightarrow}(x,k)$ may be properly normalized. Computing T and R explicitly by building the limits yields

$$\sqrt{2\pi}\lim_{x\to\infty}\psi_1^{\rightarrow}(x,k) = (-ik+1)e^{ikx} \quad \text{and} \quad \sqrt{2\pi}\lim_{x\to-\infty}\psi_1^{\rightarrow}(x,k) = (-ik-1)e^{ikx} \quad , \quad (3.14)$$

which together with equation 3.12 implies that R vanishes and

$$\begin{aligned} \psi_1^{\rightarrow}(x,k) &= \frac{-ik+\tanh(x)}{-ik-1}\frac{e^{ikx}}{\sqrt{2\pi}} = \frac{k+i\tanh(x)}{k-i}\frac{e^{ikx}}{\sqrt{2\pi}} \quad , \\ T_1 &= \frac{-ik+1}{-ik-1} = \frac{k+i}{k-i} = e^{2i\tan^{-1}(\frac{1}{k})} \quad . \end{aligned} \tag{3.15}$$

The normalization of $\psi_1^{\leftarrow}(x,k)$ may done analogously.

3.1.3 $\ell = 0, 1, 2, ...$

The aforementioned process can continue inductively for both the states and the coefficients. Hence the scattering states $|k_\ell^{\leftrightarrows}\rangle$ of a given ℓ, can be written as

$$\prod_{j=1}^{\ell} \hat{A}_j^\dagger |k_0^{\leftrightarrows}\rangle = |k_\ell^{\leftrightarrows}\rangle \quad , \tag{3.16}$$

and the transmission coefficient for the right-travelling wave yields

$$T_\ell = \prod_{j=1}^{\ell} e^{2i\tan^{-1}(\frac{j}{k})} = e^{i\delta} \quad , \tag{3.17}$$

where $\delta = \sum_{j=1}^{\ell} 2i\tan^{-1}(\frac{j}{k})$ is the phase shift. The transmission coefficient for the left-travelling wave may also be computed with this approach. This is however not necessary, as will be seen in section 3.2.1.

Further, the n^{th} bound state of the ℓ^{th} partner Hamiltonian may be found using eq. 3.8, and the relation

$$|\psi_{n,\ell}^+\rangle = |\psi_{n-1,\ell-1}^-\rangle \quad , \tag{3.18}$$

for $n = 0, \ldots, \ell - 1$. The discrete spectrum fulfils

$$\hat{\mathscr{H}}_\ell^\pm |\psi_{n,\ell}^\pm\rangle = (2n\ell - n^2)|\psi_{n,\ell}^\pm\rangle \quad . \tag{3.19}$$

Hence, the states of a given ℓ may be found gradually as shown in fig. 3.1.

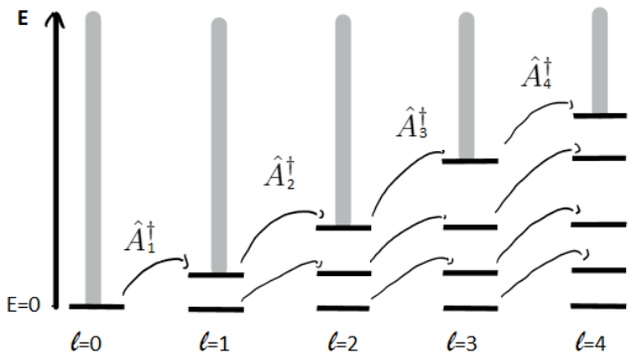

FIGURE 3.1: Sketch of the energy spectrum of the hyperbolic-system

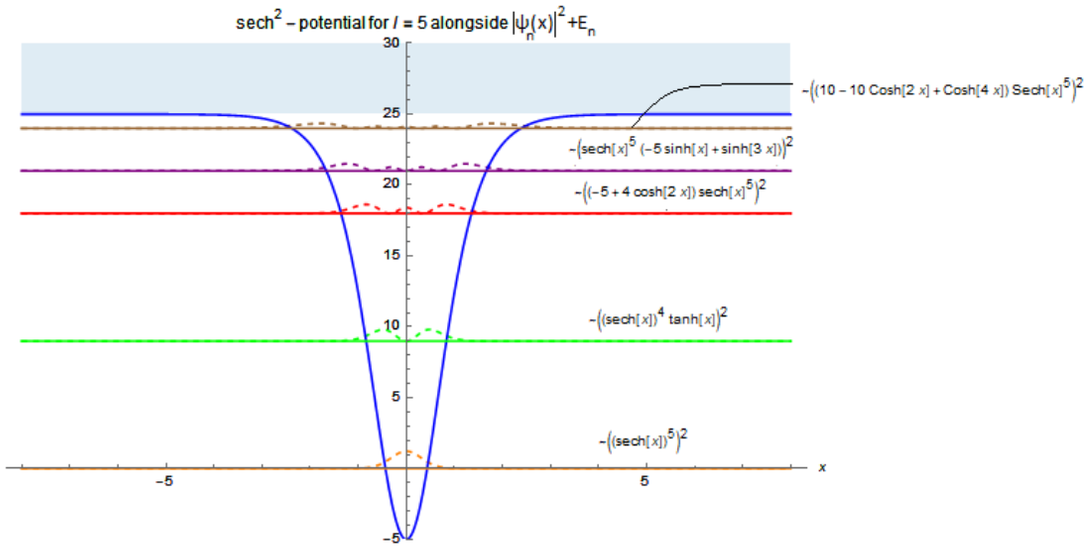

FIGURE 3.2: Potential of the $\hat{\mathscr{H}}_5^-$-system with the corresponding energy levels and bound eigenstates

The continuous spectrum yields

$$\hat{\mathscr{H}}_\ell^\pm |k_\ell^\pm\rangle = (k^2+\ell^2)|k_\ell^\pm\rangle \qquad |k_{\ell-1}^-\rangle = |k_\ell^+\rangle \quad , \tag{3.20}$$

which renders the spectrum of the system complete at last. As an example of a given spectrum for this potential consider the case of $\ell = 5$. Using eq. 3.19 the corresponding energy levels may be found, and plotted alongside the considered potential, as seen in fig. 3.2. Notice that the number of nodes increases with quantum number n. And finally the density of states $D(k) = \frac{d\delta}{dk}$ yields

$$D(k) = \frac{d\delta}{dk} = \sum_{j=1}^{\ell} \frac{-2j}{k^2 + j^2} \quad . \tag{3.21}$$

3.2 Trace of the Hamiltonian

In the following sections, the aim is to compute the canonical partition function of the system. This function is used to investigate many important properties of the system in a general framework. In this section, the relevant tools will be developed, in order to find the partition function, which is given as the trace of an analytic function of the Hamiltonian. Consider therefore such a construction for a Hamiltonian with discrete and continuous spectrum

$$\hat{\mathscr{H}}|\psi_n\rangle = E_n|\psi_n\rangle \quad \text{and} \quad \hat{\mathscr{H}}|\psi_k^{\leftrightarrows}\rangle = k^2|\psi_k^{\leftrightarrows}\rangle \tag{3.22}$$

respectively, given by (as derived in [Thi13])

$$\begin{aligned} tr(f(\hat{\mathscr{H}})) &= \sum_n f(E_n) + \iint f(k^2)\,|\psi_k^{\rightarrow}(x)|^2\,dx\,dk + \iint f(k^2)\,|\psi_k^{\leftarrow}(x)|^2\,dx\,dk \\ &:= \sum_n f(E_n) + \iint f(k^2)\,|\psi_k(x)|^2\,dx\,dk \quad . \end{aligned} \tag{3.23}$$

This expression can be simplified with the help of the so called Wronsky-determinant or Wronskian. This mathematical tool is often used when analyzing solutions of differential equations.

DEFINITION 3. *Let f and g be differentiable functions, then the Wronskian is defined as*

$$W(f,g) = f(x)(\partial_x g(x)) - (\partial_x f(x))g(x) \quad , \tag{3.24}$$

therefore, the derivative of the wronskian yields

$$W'(f,g) = f(x)g''(x) - f''(x)g(x) \quad . \tag{3.25}$$

In order to see how the Wronskian may be of assistance simplifying the trace discussed above, consider the solution $\psi(x)$ of a Schrödinger equation of the form

$$(-\frac{d^2}{dx^2} + V(x))\psi(x) = E\psi(x) \quad . \tag{3.26}$$

For a scattering state, both the eigenstate $\psi(x)$ and the eigenvalue E depend on k. Therefore, the derivative of equation 3.26 with respect to k yields in this case

$$-\dot{\psi}''(x,k) + V\dot{\psi}(x,k) = \dot{E}\psi(x,k) + E\dot{\psi}(x,k) \quad , \tag{3.27}$$

where the dot denotes the derivatives with respect to k. $\psi(x,k)$ maybe assumed to be differentiable with respect to both arguments (x, k), the former as a solution of a second order ODE and the latter because of the smoothness inherent of a physical system in regards to its energy.

Using this, eq. 3.25 for $\dot{\psi}(x,k)$ and $\psi^*(x,k)$ yield

$$W'(\dot{\psi}(x,k), \psi^*(x,k)) = \dot{\psi}(x,k)\psi^{*\prime\prime}(x,k) - \dot{\psi}''(x,k)\psi^*(x,k) \quad . \tag{3.28}$$

Replacing the second derivatives in eq. 3.28 using equations 3.26 and 3.27 yields

$$W'(\dot{\psi}, \psi^*) = \dot{\psi}\psi^*(V-E) - \dot{\psi}\psi^*(V-E) + \dot{E}\psi\psi^* = \dot{E}|\psi|^2 \quad . \tag{3.29}$$

Using this outcome, equation 3.23 may be simplified,

$$tr(f(\hat{\mathscr{H}})) = \sum_n f(E_n) + \int dk\, f(k^2)\frac{W(\dot{\psi}, \psi^*)|_{-\infty}^{\infty}}{\dot{E}} \quad . \tag{3.30}$$

This analysis avoids an integration, and replaces it by a construction dependant on derivatives of eigenstates at large x-values. This alone may be very helpful, but due to the properties of scattering states, the Wronskian can be further simplified.

3.2.1 General Computation of the Wronskian

For the general computation of the Wronskian, it is necessary to consider both the right (eq. 3.12) and left (eq. 3.13) travelling components of the scattering state. A more thorough

examination of this technique among a deeper treatment of the quantum scattering theory can be found in [Koe08]. The use of infinity in this consideration allows for a better mathematical model, however it does no refer to the actual infinity, but rather to a point in space that lies orders of magnitude far away from the considered region. The discussion about the actual physical existence of infinity lies beyond the scope of this thesis however interesting it might be. Therefore let the system lie in the center of a box of length L. For readability, set the x-value at one end of the box (i.e. at "infinity") $x_\infty = x$ and the x-value at the other end of the box (i.e. "minus infinity") $x_{-\infty} = y$. Then $L = x - y$, and the Wronskian of $\dot{\psi}, \psi^*$ for the right travelling wave would be given by

$$\begin{aligned} 2\pi W(\dot{\psi_\rightarrow}, \psi^*_\rightarrow)|^\infty_{-\infty} &= 2(k(L - |R|^2(x+y)) \\ &- Re(R)\sin(2ky) + Im(R)\cos(2ky) - ik(R^*\dot{R} + T^*\dot{T})) \quad , \end{aligned} \tag{3.31}$$

The Wronskian for the left travelling wave-function yields,

$$\begin{aligned} 2\pi W(\dot{\psi_\leftarrow}, \psi^*_\leftarrow)|^\infty_{-\infty} &= 2(k(L + |\overline{R}|^2(x+y)) \\ &+ Re(\overline{R})\sin(2ky) + Im(\overline{R})\cos(2ky) - ik(\overline{R}^*\dot{\overline{R}} + T^*\dot{T})) \end{aligned} \tag{3.32}$$

To find a link between the coefficients of the right and left travelling wave-function, notice that for states with the same energy, the Wronskian is constant. Therefore, it holds

$$\lim_{x\to-\infty} \frac{\pi}{i} W(\psi_\leftarrow, \psi_\rightarrow) = \lim_{x\to\infty} \frac{\pi}{i} W(\psi_\leftarrow, \psi_\rightarrow) = k\bar{T} = kT \quad \Rightarrow \quad T = \bar{T} \quad , \tag{3.33}$$

and analogously,

$$\lim_{x\to-\infty} \frac{\pi}{i} W(\psi_\leftarrow, \psi^*_\rightarrow) = \lim_{x\to\infty} \frac{\pi}{i} W(\psi_\leftarrow, \psi^*_\rightarrow) = k\bar{T}R^* = -kT^*\bar{R} \quad . \tag{3.34}$$

Since $T = \bar{T}$ and it can written as $T = |T|e^{i\delta}$, follows for R,

$$\bar{R} = -e^{2i\delta}R^* \quad . \tag{3.35}$$

Furthermore, the **Riemann-Lebesgue Lemma** states, that the integral of a rapidly oscillating function will approach zero as the frequency approaches infinity, as is the case for terms like $\sin(2ky)$ in both Wronskians. This lemma and its proof can be found for example in [Nai18].

With this, and the relations between transmission and reflection coefficients, the Wronskians can be reduced to

$$2\pi W(\dot{\psi_{\rightarrow}}, \psi^*_{\rightarrow})|^{\infty}_{-\infty} = 2(k(L-|R|^2(x+y)) - ik(R^*\dot{R} + T^*\dot{T})) + \dots \quad (3.36)$$

$$2\pi W(\dot{\psi_{\leftarrow}}, \psi^*_{\leftarrow})|^{\infty}_{-\infty} = 2(k(L+|\overline{R}|^2(x+y)) - ik(\overline{R}^*\dot{\overline{R}} + T^*\dot{T})) + \dots \quad . \quad (3.37)$$

In order to find the Wronskian of both the left and right travelling wave-function, it is necessary to realize that,

$$|T|^2 + |R|^2 = 1 \quad \Rightarrow |T||\dot{T}| + |R||\dot{R}| = 0 \quad . \quad (3.38)$$

Together this yields the Wronskian of the general scattering wave function,

$$\pi W(\dot{\psi}, \psi^*)|^{\infty}_{-\infty} = 2k(L + \dot{\delta}) + \dots \quad . \quad (3.39)$$

This outcome allows to compute the canonical partition function of the considered system analytically.

3.3 Computation of the Canonical Partition Function

Combining equations 3.30 and 3.39 for the Hamiltonian treated above, it is possible to find the canonical partition function of the system,

$$tr(e^{-\beta\hat{\mathscr{H}}^-_{\ell}}) = \sum_{n=0}^{\ell-1} e^{-\beta(2n\ell - n^2)} + \int_0^{\infty} dk\, \frac{e^{-\beta(k^2+l^2)}}{\dot{E}} \frac{2k}{\pi}(L + \dot{\delta}) \quad , \quad (3.40)$$

where $\beta = 1/k_B T$. Since $E = k^2$, the equation above becomes

$$tr(e^{-\beta\hat{\mathscr{H}}^-_{\ell}}) = \sum_{n=0}^{\ell-1} e^{-\beta(2n\ell - n^2)} + \int_0^{\infty} dk\, e^{-\beta(k^2+\ell^2)} \frac{1}{\pi}(L + \dot{\delta}) \quad . \quad (3.41)$$

Together with equation 3.21, it yields

$$tr(e^{-\beta\hat{\mathscr{H}}^-_{\ell}}) = \sum_{n=0}^{\ell-1} e^{-\beta(2n\ell - n^2)} + \frac{e^{-\beta\ell^2}}{\pi}\left[L\int_0^{\infty} dk\, e^{-\beta k^2} - \sum_{j=1}^{\ell} 2j \int_0^{\infty} dk\, \frac{e^{-\beta k^2}}{k^2 + j^2}\right] \quad . \quad (3.42)$$

On the one hand, the first integral has the form of a Gauss integral over $\mathbb{R}^+$ and thus yields $\sqrt{\pi}/2$. On the other hand, the second may be computed as follows. Let I denote the second integral above. Then,

$$I = \int_0^\infty dk\, \frac{e^{-\beta k^2}}{k^2+j^2} = e^{\beta j^2} \int_0^\infty dk\, \frac{e^{-\beta(k^2+j^2)}}{k^2+j^2} = e^{\beta j^2} \int_\beta^\infty d\beta' \int_0^\infty dk\, e^{-\beta'(k^2+j^2)} \quad , \tag{3.43}$$

whereby a change of order of integration was performed. With the same argument as before, the integral yields

$$I = \frac{e^{\beta j^2}\sqrt{\pi}}{2} \int_\beta^\infty d\beta'\, \frac{e^{-\beta' j^2}}{\sqrt{\beta'}} \quad . \tag{3.44}$$

On substituting $\eta = \sqrt{\beta'}j$,

$$I = \frac{e^{\beta j^2}\sqrt{\pi}}{2}\frac{\sqrt{\pi}}{j} \int_{\sqrt{\beta}j}^\infty d\eta\, \frac{2e^{-\eta^2}}{\sqrt{\pi}} := e^{\beta j^2}\frac{\pi}{2j}\mathrm{erfc}(\sqrt{\beta}j) \quad , \tag{3.45}$$

which yields for the partition function,

$$tr(e^{-\beta\hat{\mathscr{H}}_\ell^-}) = \sum_{n=0}^{\ell-1} e^{-\beta(2n\ell-n^2)} + \frac{Le^{-\beta\ell^2}}{2\sqrt{\pi\beta}} - \sum_{j=1}^{\ell} e^{-\beta(\ell^2-j^2)}\mathrm{erfc}(\sqrt{\beta}j) \quad , \tag{3.46}$$

This outcome is plotted for various values of ℓ in fig. 3.3. Notice, that as β approaches infinity (small temperatures), the partition function tends towards a constant, namely towards the number one. This may be explained by arguing, that for small temperatures, the states of the system tend to fall towards the ground energy level. Since the considered system is that of unbroken supersymmetry, the ground energy is set to zero $E_{\ell,0} = 0$. This yields for $\beta \to \infty$,

$$tr(e^{-\beta\hat{\mathscr{H}}_\ell^-}) = \underbrace{\langle\psi_0|(e^{-\beta\hat{\mathscr{H}}_\ell^-})|\psi_0\rangle}_{e^{-\beta E_{\ell,0}}} + \underbrace{\sum_{n=1}^{\ell-1} e^{-\beta(2n\ell-n^2)} + \frac{Le^{-\beta\ell^2}}{2\sqrt{\pi\beta}} - \sum_{j=1}^{\ell} e^{-\beta(\ell^2-j^2)}\mathrm{erfc}(\sqrt{\beta}j)}_{\xrightarrow{\beta\to\infty} 0} = 1 \quad . \tag{3.47}$$

The plot also shows, that for big ℓ, the system assumes the ground state faster, as β grows.

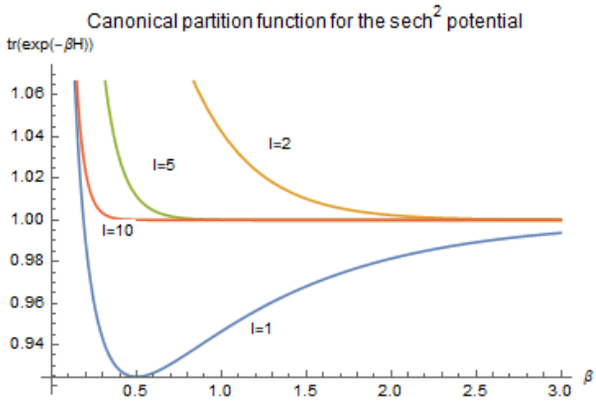

FIGURE 3.3: graphic representation of the partition function for ℓ=1,2,5,10

CHAPTER 4

Periodic Case

In this chapter, the general case of $m \neq 1$ will be considered. In order to properly compute the band-edge-eigenstates, special focus will be given to the case $\ell = 1$.

4.1 Spectrum of the Elliptical System

The spectrum of a potential well consists often of discrete bounded energies and of continuous scattering energies. Because of the periodic nature of the potentials considered in this chapter, the structure of the spectrum transforms to continuous bounded energy bands and continuous unbounded energies. This change occurs due to the interaction of the bound states across barriers. The Bloch condition represents a powerful tool to explore the properties of periodic potentials. In one dimension, this condition is given by

$$\psi(x + L) = e^{ikL}\psi(x) \quad , \tag{4.1}$$

where L denotes the length of the period of the potential. The function $\psi(x)$ is known as a Bloch fucntion or Bloch solution.

4.1.1 Ground State

In this section, periodic potentials will be analyzed using SUSY quantum mechanics. Being periodic, these potentials do not require their eigenstates to be normalized over the complete space, but only over the period L. This renders the discussion about ground states at the end of section 2.2.3 invalid. In fact, a periodic supersymmetric system may have an energy

degeneracy at the ground level.

Consider the superpotential for a given m,

$$\sigma = \ell m \frac{\mathrm{sn}(x,m)\mathrm{cn}(x,m)}{\mathrm{dn}(x,m)} = -\ell \frac{\mathrm{dn}(x,m)'}{\mathrm{dn}(x,m)} \quad . \tag{4.2}$$

The potentials would be therefore,

$$\begin{aligned} V_\ell^\pm(x,m) &= \sigma^2 \pm \sigma' \\ &= \ell^2 \frac{\mathrm{dn}'(x,m)^2}{\mathrm{dn}(x,m)^2} \mp \ell\left(\frac{\mathrm{dn}''(x,m)}{\mathrm{dn}(x,m)} - \frac{\mathrm{dn}'(x,m)^2}{\mathrm{dn}(x,m)^2}\right) \\ &= m((\ell^2 \mp \ell)\mathrm{sn}(x,m)^2 + (\ell^2 \pm \ell)\mathrm{cd}(x,m)^2 - \ell^2) \quad . \end{aligned} \tag{4.3}$$

This structure corresponds to the wider class of potentials known as associated Lamé potentials. The periodic properties of these potentials are given by the functions $\mathrm{sn}(x,m)$ and $\mathrm{cn}(x,m)$ respectively (in the case of $\mathrm{cd}(x,m) = \frac{\mathrm{cn}(x,m)}{\mathrm{dn}(x,m)}$, the elliptic cosine determines the period because its period is twice that of the elliptic delta). Since both $\mathrm{sn}(x,m)$, and $\mathrm{cn}(x,m)$ have a period on the real axis of $4K(m)$, and the functions change signs every $2K(m)$, the period of the potential becomes $L = 2K(m)$. The function $K(m)$ denotes the complete elliptic integral and characterizes the period of the Jacobi elliptic functions. More information regarding the elliptic integrals, as well as the Jacobi elliptic functions can be found in [Sch15], [WW96], [Jac29] or in the Appendix A.

For the considered potentials $V^\pm$, the corresponding Hamiltonians would be given by

$$\hat{\mathscr{H}}_\ell^\pm = -\partial_x^2 + V_\ell^\pm(x,m) \quad . \tag{4.4}$$

Using the addition theorem for the elliptic sine (cf. A.20), is possible to show that $\mathrm{sn}(x,m)^2 = \mathrm{cd}(x+K(m),m)^2$. Therefore the potentials are linked via $V(x)_\ell^+ = V(x+K(m))_\ell^-$ and the systems described by the partner Hamiltonians are equivalent to each other. Hence, the partner Hamiltonians are self-isospectral and it suffices to consider one of them, here $\hat{\mathscr{H}}_\ell^-$. With $\hat{A}_\ell = \partial_x + \sigma_\ell$ the Hamiltonians become

$$\hat{\mathscr{H}}_\ell^- = \hat{A}_\ell^\dagger \hat{A}_\ell \qquad \text{and} \qquad \hat{\mathscr{H}}_\ell^+ = \hat{A}_\ell \hat{A}_\ell^\dagger \quad . \tag{4.5}$$

The ground state $\psi_{0,\ell}$ can be found by considering the action of $\hat{A}_\ell$ on it. Since for all ℓ it holds $\hat{A}_\ell \psi^-_{0,\ell} = 0$, the following differential equation arises for the ground state:

$$(\partial_x - \ell \frac{\mathrm{dn}'(x,m)}{\mathrm{dn}(x,m)})\psi^-_{0,\ell} = 0 \quad , \tag{4.6}$$

for which

$$\psi^-_{0,\ell} = C\mathrm{dn}(x,m)^\ell \tag{4.7}$$

is a solution with C an undetermined constant. As stated at the beginning of the section, both ground states may be allowed, even though

$$\psi^-_{0,\ell} \sim \frac{1}{\psi^+_{0,\ell}} \tag{4.8}$$

holds as seen before. Incidentally, the equation above implies that

$$\psi^+_{0,\ell} = C'\mathrm{dn}(x,m)^{-\ell} \quad , \tag{4.9}$$

for another constant C'.

4.1.2 ℓ=1

On the one hand, consistency dictates to explore the case of $\ell = 0$ first, however, the fact remains that for this case the superpotential vanishes. Therefore the system does not differ from the one discussed in 3.1.1, except for the fact, that as stated above, both ground states may exist.

For $\ell = 1$, the partner Hamiltonians become

$$\hat{\mathscr{H}}_1^- = -\frac{d^2}{dx^2} + m(2\mathrm{sn}(x,m)^2 - 1) \tag{4.10}$$

and

$$\hat{\mathscr{H}}_1^+ = -\frac{d^2}{dx^2} + m(2\mathrm{cd}(x,m)^2 - 1) \quad . \tag{4.11}$$

Because the hyperbolic case yields for $\ell = 1$ a bound state at $E = 0$, and scattering states above $E = 1$, (see equations 3.19 and 3.20), the expectation for this system, is a bounded energy band with one edge at $E = 0$, and unbounded energies above $E = 1$. Therefore, the

other bounded energy band edge ought to be below $E = 1$.

In order to find the eigenstates, consider, in accordance to Bloch´s condition (eq. 4.1), that there exist states in the spectrum that fulfil,

$$\psi(x + L) = \psi(x) \quad \text{and} \quad \psi(x + L) = -\psi(x) \quad . \tag{4.12}$$

Since $L = 2K(m)$, possible eigenfunctions which fulfil the condition above ought to have either a period of L, or $2L$. Any of the Jacobi elliptic functions on its own fulfils at least one of the aforementioned conditions. Moreover, all elliptic functions also solve a characteristic non linear second order differential equation of the form

$$\frac{d^2\psi(x)}{dx^2} = \alpha(m)\psi(x)^3 + \beta(m)\psi(x) \quad . \tag{4.13}$$

Hence it is a good Ansatz to consider some elliptical function $\mathrm{zn}(x, m)$, and its second derivative, since its coefficients $\alpha(m)$ and $\beta(m)$ are characteristic of the function. Letting $\hat{\mathscr{H}_1^-}$ operate on to $\mathrm{zn}(x, m)$ yields,

$$(-\frac{d^2}{dx} + V^-(x, m))\mathrm{zn}(x, m) = (-\alpha(m)\mathrm{zn}(x, m)^2 - \beta(m) + m(2\mathrm{sn}(x, m)^2 - 1))\mathrm{zn}(x, m) \quad . \tag{4.14}$$

In order to solve the Schrödinger equation, some $\alpha(m)$ and $\beta(m)$ must exist such that,

$$-\alpha(m)\mathrm{zn}(x, m)^2 - \beta(m) + m(2\mathrm{sn}(x, m)^2 - 1) = E \quad . \tag{4.15}$$

As can be seen in the mathematical literature (e.g. [Sch15]) or in the table A.3, the known groundstate $\mathrm{dn}(x, m)$ has coefficients $\alpha = -2$, and $\beta = 2 - m$. This yields the expected lower band edge at $E = 0$.

Plugging in different coefficients and its respective functions, the expected spectrum is realized, and the band-edge-eigenstates are found to be $\mathrm{dn}(x, m)$, $\mathrm{cn}(x, m)$ and $\mathrm{sn}(x, m)$, with an energy band going from $E = 0$ to $E = 1 - m$, a band gap, and continuous energies from $E = 1$ respectively (see fig.4.1 as well as table 4.1). In order to find the remaining states, a more formal solution of the eigenvalue problem of the Hamiltonian 4.10 is necessary. This problem can be expressed by

E	ψ^-	**Period**
0	$\mathrm{dn}(x,m)$	$2K(m)$
$1-m$	$\mathrm{cn}(x,m)$	$4K(m)$
1	$\mathrm{sn}(x,m)$	$4K(m)$

TABLE 4.1: Eigenvalues and eigenstates for the potential $V(x) = m(2\mathrm{sn}(x,m)^2 - 1)$.

$$\psi(x)'' = (2m \cdot \mathrm{sn}(x,m)^2 - m - E)\psi(x) \quad , \tag{4.16}$$

which is known in the mathematical literature, as a special case of the Lamé differential equation, the solution of which is presented in [WW96] and is sketched in the appendix B2. In the considered case of $\ell = 1$ the solution is given by the following independent functions (cf.B.9, B.10),

$$\psi_\pm(x) = \frac{H(x \pm \tilde{\alpha}(E))}{\Theta(x)} e^{\mp x Z(\tilde{\alpha}(E))} \quad , \tag{4.17}$$

where $\tilde{\alpha}$ is chosen to satisfy the condition

$$\begin{aligned} &(\mathrm{cn}(\tilde{\alpha},m)\mathrm{ds}(\tilde{\alpha},m))^2 - \mathrm{ns}(\tilde{\alpha},m)^2 = -m - E \\ &\xRightarrow[\text{properties of J. elliptic funct.(cf. Tab.A.1)}]{} \mathrm{dn}(\tilde{\alpha},m)^2 = E \quad . \end{aligned} \tag{4.18}$$

Using these solutions, it is possible to find the dispersion relation of this system analytically. For this, apply the Bloch condition 4.1 to the eigenstates described above. Using the properties of the Jacobi Zeta, Theta and Eta functions (discussed in [Jac29] and in the appendix B1) the Bloch condition yields,

$$\frac{H(x+L \pm \tilde{\alpha}(E))}{\Theta(x+L)} e^{\mp(x+L)Z(\tilde{\alpha}(E))} = e^{ikL} \cdot \frac{H(x \pm \tilde{\alpha}(E))}{\Theta(x)} e^{\mp x Z(\tilde{\alpha}(E))} \quad . \tag{4.19}$$

Further, due to the periodicity properties of H and Θ (cf. B.7), this equation yields

$$\begin{aligned} -e^{\mp(x+L)Z(\tilde{\alpha}(E))} &= e^{ikL} \cdot e^{\mp x Z(\tilde{\alpha}(E))} \\ \Rightarrow 1 &= -e^{ikL \mp L Z(\tilde{\alpha}(E))} \quad . \end{aligned} \tag{4.20}$$

This implies for an $n \in \mathbb{Z}$

$$k_\pm = \frac{(2n+1)\pi}{L} \pm i Z(\tilde{\alpha}(E)) \quad . \tag{4.21}$$

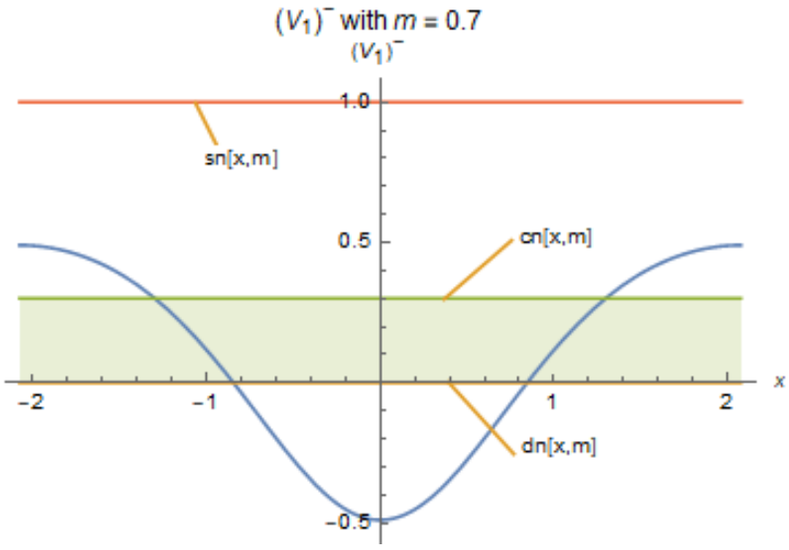

FIGURE 4.1: Periodic potential for $\ell = 1$ and $m = 0.7$ plotted alongside its allowed energies. The Energies of the band-edges are connected to their corresponding eigenstates.

Constraining k to the Brillouin zone (at the boundary of which $k_\pm = \frac{\pi}{L}$), further simplifies the dispersion relation. With this constrain, $k_\pm$ yields

$$k_\pm = \mp\frac{\pi}{L} \pm iZ(\tilde{\alpha}(E)) \quad , \tag{4.22}$$

a result that can also be found in [DF98]. As an example consider the dispersion relation belonging to the solution ψ_- as depicted in fig. 4.2. Notice the band gap between $E = 1 - m = 0.7$ and $E = 1$, and how the imaginary part of k_- vanishes everywhere except in this region. The density of states $D(E)$ can be thought of as the density of momenta per energy, and can therefore be written as

$$\begin{aligned} D_\pm(E) =& \frac{dk_\pm}{dE} \\ =& \pm i\frac{\partial Z(\tilde{\alpha})}{\partial\tilde{\alpha}}\frac{\partial\tilde{\alpha}}{\partial E} \\ =& \pm i\left(\mathrm{dn}(\tilde{\alpha}) - \frac{\mathbb{E}(K(m),m)}{K(m)}\right)\frac{\partial\tilde{\alpha}}{\partial E} \\ =& \mp\frac{i}{2(E+m-1)}\left(\sqrt{E} - \frac{\mathbb{E}(K(m),m)}{\sqrt{E}K(m)}\right)\mathrm{cs}(\tilde{\alpha}) \quad . \end{aligned} \tag{4.23}$$

Where $\mathbb{E}(x,m)$ denotes the elliptic integral of the second kind. As can be seen in fig. 4.3, the general behaviour of the $D_-(E)$ resembles that of the (non relativistic) free particle density

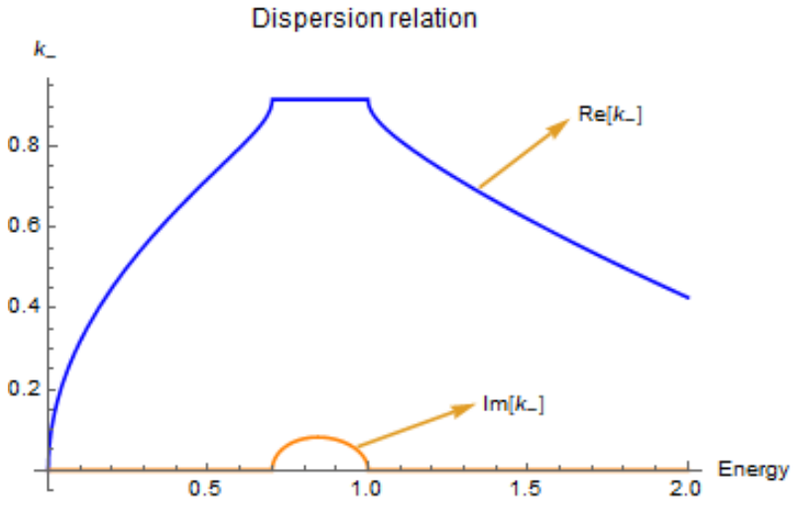

FIGURE 4.2: Real and imaginary parts of the dispersion relation $k_{-}(E)$ for the potential $V = m(2\mathrm{sn}(x,m)^2 - 1)$ with $m = 0.3$.

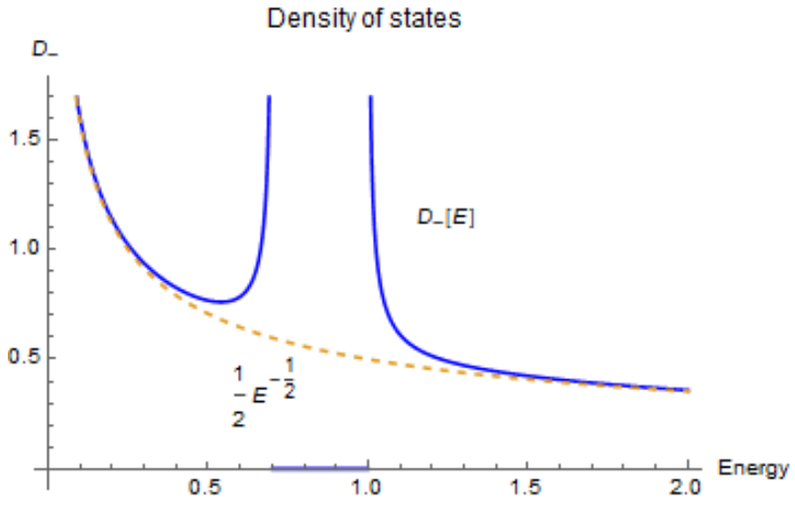

FIGURE 4.3: Density of states D_{-} for $V = m(2\mathrm{sn}(x,m)^2 - 1)$ with $m = 0.3$

of states ($E^{-\frac{1}{2}}/2$), differing by the non-continuity found in energies belonging to the band gap. As expected, in this region the density of states vanishes.

4.1.3 $\ell = 2$

The potential V^- for $\ell = 2$ becomes

$$\begin{aligned} V_2^-(x,m) =& m(6\mathrm{sn}(x,m)^2 + 2\mathrm{cd}(x,m)^2 - 4) \\ =& 2m(3\mathrm{sn}(x,m)^2 + \mathrm{cd}(x,m)^2 - 2) \end{aligned} \quad , \tag{4.24}$$

which belongs to the class of associated Lamé potentials. As such the solution discussed in [WW96] does not help in this case. Nevertheless, an analytic approach does exist, as is sketched in [KS04]. Consider the Schrödinger eq. for this system,

$$-\frac{d^2}{dx^2}\psi(x) + V_2^-\psi(x) = E\psi(x) \quad . \tag{4.25}$$

Substituting $\psi(x) = \mathrm{dn}(x,m)^2 z(x)$, and $x = F(t,m)$ yields an equation known in the mathematical literature as a special case of the Ince equation.

$$(1 + A\cos(2t))z''(t) + B\sin(2t)z'(t) + Cz(t) = 0 \quad , \tag{4.26}$$

Where

$$A = \frac{m}{m-2} \quad , \quad B = \frac{5m}{m-2} \quad , \quad C = \frac{E}{2-m} \quad . \tag{4.27}$$

Here, $F(t,m)$ denotes the incomplete elliptic integral and transforms the elliptic function into a trigonometric one. For this equation, the band edge eigenfunctions are known, and can be retrieved to find the eigenstates of the Schrödinger equation. These are tabulated in table 4.2. Notice the similarities between ψ_1^- and ψ_4^- as well as between ψ_2^- and ψ_3^-, namely that the function inside the parenthesis is shifted by a constant dependent on m. A similar shift can be found in the energies. Figure 4.4 shows the considered potential, as well as its energy-spectrum. Notice both the first band of allowed energies as well as the second energy band gap being barely visible in the plot. The choice of $m = 0.7$ leads to a spectrum that can be approximated as having a ground state at $E = 0$, and a continuous spectrum above $E \approx 1.5$.

n	**E**	ψ_n^-	**Period**
0	0	$\mathrm{dn}(x,m)^2$	$2K(m)$
1	$5-3m-2\sqrt{4-3m}$	$\mathrm{cd}(x,m)(3m\cdot\mathrm{sn}(x,m)^2-2-\sqrt{4-3m})$	$4K(m)$
2	$5-2m-2\sqrt{4-5m+m^2}$	$\mathrm{sd}(x,m)(3m\cdot\mathrm{sn}(x,m)^2-2-m-\sqrt{4-5m+m^2})$	$4K(m)$
3	$5-2m+2\sqrt{4-5m+m^2}$	$\mathrm{sd}(x,m)(3m\cdot\mathrm{sn}(x,m)^2-2-m+\sqrt{4-5m+m^2})$	$4K(m)$
4	$5-3m+2\sqrt{4-3m}$	$\mathrm{cd}(x,m)(3m\cdot\mathrm{sn}(x,m)^2-2+\sqrt{4-3m})$	$4K(m)$

TABLE 4.2: Eigenvalues and eigenstates for the potential $V(x)=2m(3\mathrm{sn}(x,m)^2+\mathrm{cd}(x,m)^2-2)$.

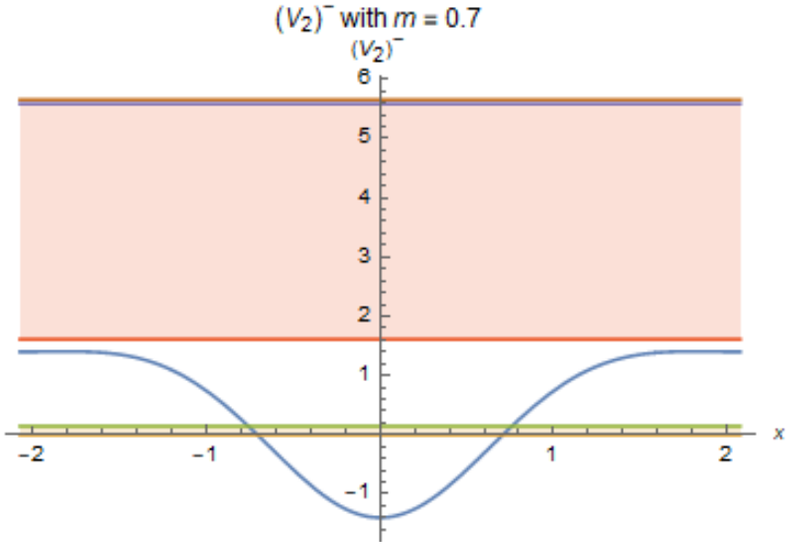

FIGURE 4.4: Periodic potential for $\ell=2$ and $m=0.7$, plotted alongside its allowed energies

4.1.4 $\ell = 0, 1, 2, \ldots$

The general form of the Schrödiner equation, with the potential of eq. 4.3, may be transformed into a more general form of Ince equation, by generalizing the substitutions done in the section above. Substituting $\psi(x)=\mathrm{dn}(x,m)^\ell z(x)$, and $x=F(t,m)$ leads to the same Ince equation given above (eq.4.26), however the coefficients have to be redefined.

$$A=\frac{m}{m-2}\quad,\quad B=\frac{(2\ell+1)m}{m-2}\quad,\quad C=\frac{E}{2-m}\quad. \tag{4.28}$$

As already stated, the solutions for the band edges of this equation are known, and may be found in the mathematical literature (e.g. in [MW13]).

4.2 Numerical Generalization

In order to analyze other potentials, the knowledge of the value of the energy band edges is very helpful. To analyze a given periodic potential, and find these properties, the use of a more general theory of differential equations specialized in periodic potentials is needed. Such a theory is known as Floquet-Lyapunov theory, and allows for a numerical approach to this topic.

4.2.1 Fundamentals of Floquet-Lyapunov Theory

Diving into the proofs needed to fully understand this theory, goes beyond the scope of this thesis. However the formal mathematical approach may be found in [Kuc12]. For the purposes of this chapter, it suffices to understand the basic theorems and what they imply, as was done in [Kuc16].

A linear system of ordinary differential equations with constant coefficients

$$\frac{d}{dx}\vec{\phi}(x) = B\vec{\phi}(x) \quad , \tag{4.29}$$

has, according to **Euler´s Theorem**, solutions $\phi_\lambda(x)$ of the form

$$\phi_\lambda(x) = e^{i\lambda x}\sum_{j\in\mathbb{Z}^+} p_j x^j \quad , \tag{4.30}$$

or linear combinations of them. Here is $\vec{\phi}(x) \in \mathbb{C}^d$, B a $d \times d$ constant Matrix, $i\lambda$ an eigenvalue of B, and the sum is finite. If the matrix B does not have Jordan blocks, only the term $j = 0$ is present in 4.30.

Consider now a similar system of ordinary differential equations,

$$\frac{d}{dx}\vec{\phi}(x) = \Upsilon(x)\vec{\phi}(x) \quad , \tag{4.31}$$

where $\Upsilon(x) = \Upsilon(x + L)$ is a $d \times d$ L-periodic Matrix. Such a system has d independent solutions that may be arranged in a canonical way, namely in the so-called *fundamental solution*.

DEFINITION 4. *A fundamental solution $\Phi(x)$ of a linear system of ODE´s (see eq. 4.31) is a $d \times d$ matrix for which each column is an independent solution of the system and fulfils the condition*

$$\Phi(0) = \mathbb{1} \quad . \tag{4.32}$$

Notice that the aforementioned condition implies that for all x, $\det(\Phi) = 1$.
With this, the **Floquet-Theorem** may be properly stated. For an ODE such as the one presented in eq. 4.31, there exists a constant matrix C and a L-periodic matrix function $P(x)$ such that the fundamental solution is given by

$$\Phi(x) = P(x)e^{Cx} \quad . \tag{4.33}$$

This implies that $P(0) = \mathbb{1}$. Notice that, due to the periodicity of $P(x)$, for $x = L$ the fundamental solution becomes $\Phi(L) = e^{CL}$. At this point, it is convenient to introduce the monodromy matrix M as

$$M := \Phi(L) = e^{CL} \quad . \tag{4.34}$$

This definition implies that the monodromy matrix retains a lot of properties of the fundametal solution, like for example the determinant. Therefore the eigenvalues z_i of M fulfil

$$\prod_i z_i = 1 \quad . \tag{4.35}$$

This eigenvalues are known as Floquet multipliers. A corollary of the Floquet-Theorem together with Euler's Theorem states what essentially amounts to a generalized version of the Bloch condition: it expresses that any solution of eq. 4.31 is a linear combination of Floquet (or Floquet-Bloch) solutions,

$$\phi_k(x) = e^{ikx} \sum_{j \in \mathbb{Z}^+} p_j(x) x^j \quad , \tag{4.36}$$

where the $p_j(x)$ are L-periodic functions and the sum is finite. It also states, that the eigenvalues of the monodromy matrix have the form $z_j = e^{ik_j L}$, and that if M does not have Jordan blocks, only the term for $j = 0$ is present in 4.36.

Applying this formalism to the Schrödinger equation relies upon the fact, that any higher order differential equation may be reduced to a system of coupled first order differential equations.

4.2.2 Floquet-Lyapunov Theory in Quantum Mechanics

For the canonical Floquet-Lyapunov Theory, a system of first order linear ODE's is needed. Consider a Schrödinger equation of the form

$$(-\frac{d^2}{dx^2} + V(x))\psi(x,E) = E\psi(x,E) \quad , \tag{4.37}$$

where $V(x)$ is a L-periodic potential. Introducing the following substitution

$$\psi(x,E) = \phi_1(x,E) \qquad \text{and} \qquad \psi'(x,E) = \phi_2(x,E) \quad , \tag{4.38}$$

yields

$$\frac{d}{dx}\begin{pmatrix}\phi_1(x,E)\\ \phi_2(x,E)\end{pmatrix} = \begin{pmatrix}0 & 1\\ V(x)-E & 0\end{pmatrix}\begin{pmatrix}\phi_1(x,E)\\ \phi_2(x,E)\end{pmatrix} \quad . \tag{4.39}$$

Thus,

$$\Upsilon(x,E) = \begin{pmatrix}0 & 1\\ V(x)-E & 0\end{pmatrix} \quad , \tag{4.40}$$

and the defining condition for Υ is met.

The fundamental solution of this system may be written for solutions $\psi_{1,2}$ with boundary conditions

$$\psi_{1,2}(0,E) = \begin{cases}1\\ 0\end{cases} \quad \text{and} \quad \psi'_{1,2}(0,E) = \begin{cases}0\\ 1\end{cases} \quad . \tag{4.41}$$

Then, the monodromy matrix is given by,

$$M = \begin{pmatrix}\psi_1(L,E) & \psi_2(L,E)\\ \psi'_1(L,E) & \psi'_2(L,E)\end{pmatrix} \quad . \tag{4.42}$$

Notice that the determinant of this matrix gives rise to the Wronskian. Due to the fact that $\det(M) = 1$, $W(\psi_1,\psi_2) = 1$. Because of this togehter with the aforementioned corollary,

the Floquet multipliers may be characterized as

$$z_{1,2} = e^{\pm ikL} \quad , \tag{4.43}$$

where $k = k(E)$ is indeed the dispersion relation associated with the considered system. In order to see, that the k's of the Floquets multipliers correspond to the dispersion relation, consider the action of M^T on $\psi_{1,2}(0, E)$

$$\begin{aligned} \begin{pmatrix} \psi_1(0+L,E) \\ \psi_2(0+L,E) \end{pmatrix} =& \begin{pmatrix} \psi_1(L,E) & \psi_1'(L,E) \\ \psi_2(L,E) & \psi_2'(L,E) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ =& M^T \begin{pmatrix} \psi_1(0,E) \\ \psi_2(0,E) \end{pmatrix} \quad , \end{aligned} \tag{4.44}$$

which has the same structure as the Bloch condition. Since $\psi_{1,2}$ are linearly independent, every solution may be represented as a linear combination of them. Let the basis change in such a way, that it yields two independent Bloch solutions $\psi_\pm$. This yields

$$\begin{aligned} \begin{pmatrix} \psi_+(0+L,E) \\ \psi_-(0+L,E) \end{pmatrix} =& \begin{pmatrix} e^{ik_+L} & 0 \\ 0 & e^{ik_-L} \end{pmatrix} \begin{pmatrix} \psi_+(0,E) \\ \psi_-(0,E) \end{pmatrix} \\ :=& \tilde{M} \begin{pmatrix} \psi_+(0,E) \\ \psi_-(0,E) \end{pmatrix} \quad . \end{aligned} \tag{4.45}$$

Clearly, $\tilde{M}$ is the diagonalized matrix of the transposed monodromy matrix M^T, which has the same eigenvalues as M. As such $\tilde{M}$ has the eigenvalues of M in the diagonal. This means, that the monodromy matrix contains very relevant physical information. In order to analyze the band gaps consider the trace of M, known as the discriminant or Lyapunov function $\Delta(E)$

$$\begin{aligned} \Delta(E) := tr(M) =& \psi_1(L,E) + \psi_2'(L,E) \\ = tr(\tilde{M}) =& e^{ik_+L} + e^{ik_-L} \quad . \end{aligned} \tag{4.46}$$

So long as $k_\pm \in \mathbb{R}$ holds, the absolute value of the trace should not be greater than two. But since $\mathrm{Im}(k_\pm) \neq 0$ in the band gap (as exemplified by fig.4.22), the absolute value of the trace

becomes grater than two in this region,

$$|tr(M)| = \begin{cases} \leq 2 & \text{for allowed energies} \\ > 2 & \text{for band gaps} \end{cases} \quad . \tag{4.47}$$

Further, by using both the characteristic equation of M, and the fact that $\det(M) = 1$, it is possible to find an explicit equation for the dispersion relation. The characteristic equation yields,

$$\begin{aligned} (\psi_1 - z)(\psi_2' - z) - \psi_2\psi_1' &= 0 \\ \iff z^2 - z\Delta(E) + 1 &= 0 \\ \Rightarrow e^{ik_\pm L} = \frac{1}{2}(\Delta(E) \pm \sqrt{\Delta(E) - 4}) \quad &. \end{aligned} \tag{4.48}$$

The approach presented above can be extended to arbitrary periodic potentials, making use of a numerical solution of the corresponding Schrödinger equation with the boundary conditions presented in eq. 4.41. A more in depth look at this technique can be found in [Kuc16]. Consider the potential analyzed in the section 4.1.2 as an example. In fig. 4.5, the discriminant is plotted. Notice the expected energy gap, where the absolute value of the trace goes beyond 2. The extension of the band gap is illustrated with a red band, and extends from $E = 1 - m$ to $E = 1$.

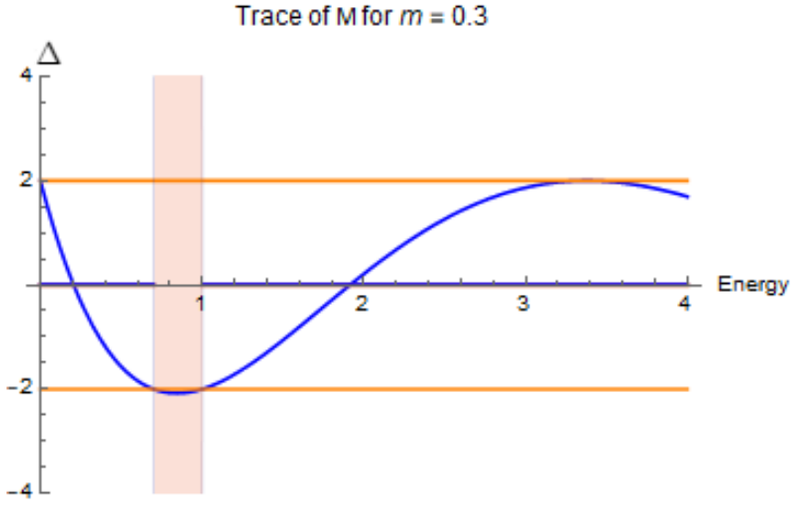

FIGURE 4.5: Discriminant for $V = m(2\mathrm{sn}(x, m)^2 - 1)$ with $m = 0.3$

4.3 Other Periodic Potentials

Using the approach described above, a qualitative investigation of other periodic potentials is possible. Since the analytic solution of the Lamé potentials is known (derived in [WW96], and sketched in the appendix B), a more qualitative understanding of them is complementary. Even though the solution is known, the computation of the energy-dependency can become very complex. Therefore, in finding the relevant energies, that is, the energies at the band edges, and knowing the structure of the general solution, the search for the edge-eigenstates may be simplified. Consider therefore a potential of the form $V_\ell = \ell(\ell+1)m \cdot \mathrm{sn}(x,m)^2 + A(E,m)$. The constant A may be chosen, such that the ground energy is at $E = 0$, using the formalism of supersymmetric quantum mechanics (see for example [OWW10]). For $\ell = 2$ the potential becomes

$$V_2 = 2(3m \cdot \mathrm{sn}(x,m)^2 - 1 - m + \sqrt{1 - m + m^2}) \quad . \tag{4.49}$$

The trace of the monodromy matrix for this system, with the conditions set in the section above, yield fig. 4.6. Here, two band gaps are detected. For $\ell = 3$ the potential is shifted to

$$V_3 = 12m \cdot \mathrm{sn}^2 - 2 - 5m + 2\sqrt{1 - m + 4m^2} \quad , \tag{4.50}$$

which yields fig. 4.7. In this case three band gaps are found. These realizations serve to illustrate the fact, that the Lamé potentials have ℓ bound bands followed by unbounded energies, as stated in [KS04].

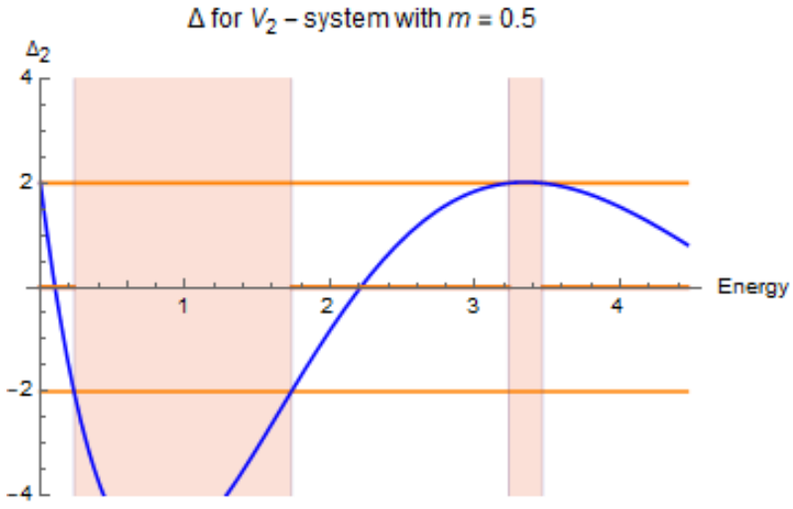

FIGURE 4.6: Discriminant for $V_2 = 2(3m \cdot \mathrm{sn}(x, m)^2 - 1 - m + \sqrt{1 - m + m^2})$ with $m = 0.5$

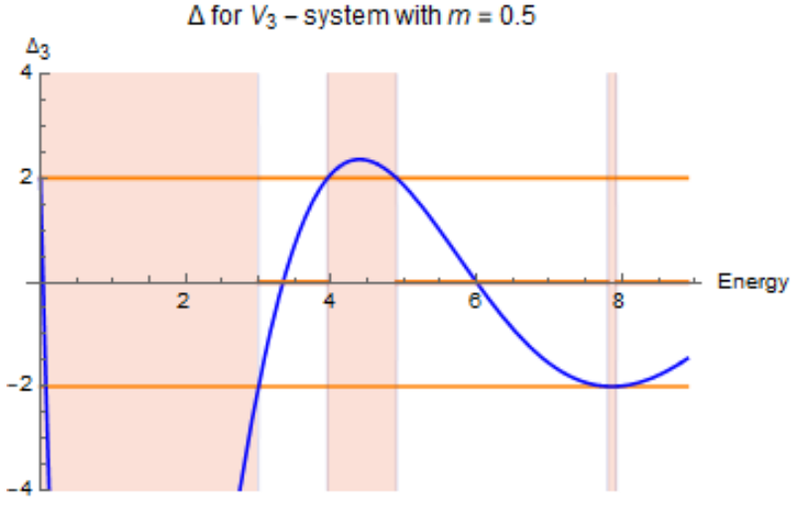

FIGURE 4.7: Discriminant for $V_3 = 12m \cdot \mathrm{sn}^2 - 2 - 5m + 2\sqrt{1 - m + 4m^2}$ with $m = 0.5$

CHAPTER 5

Conclusion

The formalism of supersymmetric quantum mechanics was successfully used to investigate non-trivial potentials. The principle class of potentials considered, potentials arsing from a superpotential $\sigma = \ell \cdot m\frac{\mathrm{sn}(x,m)\mathrm{cn}(x,m)}{\mathrm{dn}(x,m)}$, were discussed, and used to illustrate techniques which can be used on other more complex potentials. However, since both the non-periodic as well as the periodic class of supersymmetric potentials were self-isospectral, the solution of one partner system did not lead to new information about the other. The use of the Wronskian led to a simplification in the computation of physically relevant functions, such as the partition function, and to the possibility of treating any periodic potential numerically.

Since the majority of problems in quantum mechanics do not have an analytic solution, the fact that several classes of periodic potentials are solvable is uplifting and may lead to the development of better ways of modelling the electronic properties of solid materials, and thus a better understanding of this field. Furthermore, as seen in the non-periodic chapter, the potential for $m = 1$ is reflectionless. Therefore for $m \approx 1$ the arising potential may be thought of as periodic array of reflectionless potentials. This properties may be useful for technological applications, for example in the development of cables so thin, that a one dimensional approach is not out of place.

An exact dispersion relation as well as the corresponding density of states, were found for one of the cases handled, which is indeed very rare for this kind of problems. Using the Floquet-Lyapunov formalism for a given periodic potential, may allow for the numerical determination of other dispersion relations. Since it is known, that for a non relativistic particle moving in one dimension k is a function of $\sqrt{E}$, and that

$$e^{ik_{\pm}L} = \frac{1}{2}(\Delta(E) \pm \sqrt{\Delta(E) - 4}) \quad , \tag{5.1}$$

numerical methods may be able to determine the form of k. Such a technique would however be very costly in computational power. Nevertheless the knowledge gained by understanding the dispersion relation of a material may be very useful.

APPENDIX A

Introduction to the Jacobi Elliptic Functions

In this section, the Jacobi elliptic functions will be introduced from a geometric perspective, as done by [Sch15]. Special features of these functions will be discussed, as well as their notation.

A1 Geometry of the Ellipse

A way of introducing the Jacobi elliptical functions is by considering the ellipse. This approach was chosen in [Sch15], and is explored in far more detail, compared to this small introduction. In Cartesian coordinates the ellipse is given by

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \quad , \tag{A.1}$$

where $a, b > 0$. Further let the distance from the origin to the foci (on the x-axis) be denoted by c. Denote with r_1, r_2 the lines that connect each of the foci with a point p on the ellipse. Because of the characteristics of the foci, it holds,

$$r_1 + r_2 = 2a \quad . \tag{A.2}$$

Once the ellipse is normalized, it is possible to describe it with only one parameter. Usually b is normalized, and c is described as a function of a by constructing a right triangle with hypotenuse of length a, and legs of length c and 1 respectively. Doing this yields

$$c = \sqrt{a^2 - 1} \quad . \tag{A.3}$$

In order to get a single parameter, the elliptic modulus is introduced as

$$k = \frac{c}{a} = \frac{\sqrt{a^2 - 1}}{a} \quad . \tag{A.4}$$

It is sometimes preferable to use the square of the elliptic modulus $k^2 = m$ as parameter. This simplifies most of the relevant expressions, therefore, this paper will make use of the aforementioned convention.

In order to describe the ellipse with polar coordinates, not only is the angular coordinate θ of importance, but the angle-dependant radial coordinate r. Here θ denotes the angle between the x-axis and r. It is possible however, to define a new coordinate u, which describes the ellipse optimally regarding both the angle and the radius

$$du = r d\theta \quad . \tag{A.5}$$

The angular-dependence of r can be geometrically deduced, and is given by

$$r(\theta) = \frac{a}{\sqrt{\cos(\theta)^2 + a^2 \sin(\theta)^2}} \quad . \tag{A.6}$$

A2 Geometric Definitions

Analogous to the geometric definitions of the trigonometric functions based on the unit circle, it is possible to define functions based on the normalized ellipse described above (see fig. A.1). The sine-function analogue

$$\mathrm{sn}(u, m) := y \tag{A.7}$$

is called elliptic sine. For the elliptic cosine, it holds

$$\mathrm{cn}(u, m) := \frac{x}{a} \quad , \tag{A.8}$$

and because of the angle-dependent radius, it is necessary to define a third function; the elliptic delta

$$\mathrm{dn}(u, m) := \frac{r}{a} \quad . \tag{A.9}$$

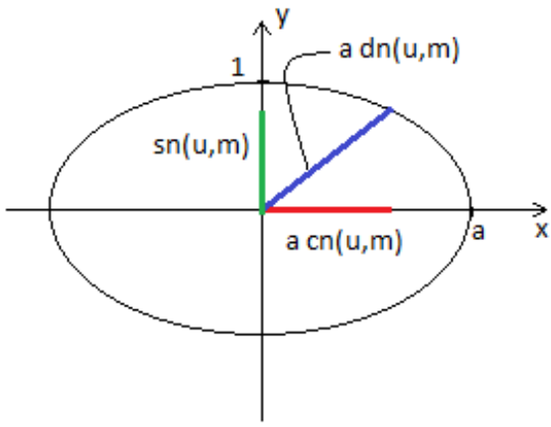

FIGURE A.1: geometric definitions of the Jacobi elliptic function using a normalized ellipse

Cartesian coordinates	**elliptic functions**
$\frac{x^2}{a^2} + y^2 = 1$	$\mathrm{sn}(u,m)^2 + \mathrm{cn}(u,m)^2 = 1$
$r^2 = x^2 + y^2$	$a^2\mathrm{cn}(u,m)^2 + \mathrm{sn}(u,m)^2 = a^2\mathrm{dn}(u,m)^2$
$m = \frac{a^2-1}{a^2}$	$\mathrm{dn}(u,m)^2 + m \cdot \mathrm{sn}(u,m)^2 = 1$

TABLE A.1: Identities of Jacobi elliptic functions and their geometric origin

base elliptic functions	**derivative**
$\mathrm{sn}(u,m)$	$\mathrm{cn}(u,m)\mathrm{dn}(u,m)$
$\mathrm{cn}(u,m)$	$-\mathrm{sn}(u,m)\mathrm{dn}(u,m)$
$\mathrm{dn}(u,m)$	$-m \cdot \mathrm{sn}(u,m)\mathrm{cn}(u,m)$

TABLE A.2: derivatives of the base Jacobi elliptic functions

This definitions immediately yield the identities found in table A.1.

Using the definitions and identities above, it is possible to find the derivatives of the base elliptic functions (see table A.2).

Building the quotients of the three base functions presented above, new elliptical functions may be defined, analogous to the tangent function as the quotient of sine and cosine in the trigonometric case. The nomenclature of a given quotient of the base elliptic functions depends entirely on the base functions that build it. To illustrate let $\mathrm{bn}(u,m)$ and $\mathrm{tn}(u,m)$ be some base elliptic function. Then

$$\frac{\mathrm{bn}(u,m)}{\mathrm{tn}(u,m)} := \mathrm{bt}(u,m) \quad . \tag{A.10}$$

Since all elliptic functions can be written as quotients of sn, cn and dn, and these base elliptic functions are related via the identities in table A.1, it is possible to show, that for any given elliptic function $\mathrm{zn}(u,m)$ it holds

$$\frac{d^2\mathrm{zn}(u,m)}{du^2} = \alpha(m)\mathrm{zn}(u,m)^3 + \beta(m)\mathrm{zn}(u,m) \tag{A.11}$$

For some $\alpha(m)$, $\beta(m)$ dependent on the parameter m, whose values are given in table A.3.

elliptic function	α	β
$\mathrm{sn}(u,m)$	$2m$	$-(1+m)$
$\mathrm{cn}(u,m)$	$-2m$	$2m-1$
$\mathrm{dn}(u,m)$	-2	$2-m$
$\mathrm{cd}(u,m)$	$2m$	$-(1+m)$
$\mathrm{sd}(u,m)$	$2m(1-m)$	$2m-1$
$\mathrm{nd}(u,m)$	$2(1-m)$	$2-m$
$\mathrm{dc}(u,m)$	2	$-(1+m)$
$\mathrm{nc}(u,m)$	$2(1-m)$	$-2m-1$
$\mathrm{sc}(u,m)$	$2(1-m)$	$2-m$
$\mathrm{ns}(u,m)$	2	$-1(1+m)$
$\mathrm{ds}(u,m)$	2	$2m-1$
$\mathrm{cs}(u,m)$	2	$2-m$

TABLE A.3: Table of coefficients of the second order ODE of Jacobi elliptical functions in the form of eq.A.11. Adapted from [Sch15].

A3 Periodic Characteristics

Because of the nature of the ellipse, the Jacobi elliptic functions ought to be periodic, and the period is bound to be dependant on the parameter m. In order to find the period, it is only needed to integrate the general coordinate around the ellipse. The table A.2 and the ellipse identities yield

$$\frac{dy}{du} = \sqrt{(1-y^2)(1-my^2)} \Rightarrow du = \frac{dy}{\sqrt{(1-y^2)(1-my^2)}} \quad . \tag{A.12}$$

This yields an expression for the coordinate u,

$$u = \int_0^y \frac{dy'}{\sqrt{(1-y'^2)(1-my'^2)}} \quad , \tag{A.13}$$

which is often written with the substitution $y = \sin(\theta)$, corresponding to the limit of m approaching zero. This substitution yields a function that links the coordinate u with the more intuitive angle θ,

$$u = F(\theta, m) := \int_0^\theta \frac{d\theta'}{\sqrt{1 - m\sin(\theta')^2}} \quad . \tag{A.14}$$

The incomplete elliptic integral $F(\theta, m)$ allows to recover trigonometric functions from the elliptic ones, since it links both the coordinates of the ellipse and of the circle. Therefore $\mathrm{sn}(F(\theta, m), m) = \sin(\theta)$.

This integral is however only well defined for $0 < y < 1$ or $0 < \theta < \pi/2$. The integral with these limits is used to define an important value, the so called complete elliptic integral $K(m)$,

$$K(m) := \int_0^1 \frac{dy}{\sqrt{(1-y^2)(1-my^2)}} \quad . \tag{A.15}$$

With the substitution done above, $K(m)$ can be written as,

$$K(m) = \int_0^{\frac{\pi}{2}} \frac{d\theta}{\sqrt{1 - m\sin(\theta)^2}} \quad . \tag{A.16}$$

Since the complete integral goes form zero to $\pi/2$, $K(m)$ only represents a fourth of the entire ellipse,

$$\int_{\textbf{Ellipse}} du = 4K(m) \quad . \tag{A.17}$$

Indeed, it holds

$$\mathrm{sn}(u, m) = \mathrm{sn}(u + 4K(m), m) \qquad \mathrm{cn}(u, m) = \mathrm{cn}(u + 4K(m), m) \quad . \tag{A.18}$$

Nonetheless, because of the symmetry of the ellipse, and the definition of the dn-function as a radius, the elliptic delta has a smaller period,

$$\mathrm{dn}(u, m) = \mathrm{dn}(u + 2K(m), m) \quad . \tag{A.19}$$

These periodic properties lead to the idea of an addition theorem for the elliptic functions. A formal derivation of such a theorem can be found in [WW96] and lies outside the scope of this introduction. the addition theorems of sn, cn and dn are given by,

$$\mathrm{sn}(u + v, m) = \frac{\mathrm{sn}(u, m)\mathrm{cn}(v, m)\mathrm{dn}(v, m) + \mathrm{sn}(v, m)\mathrm{cn}(u, m)\mathrm{dn}(u, m)}{1 - m \cdot \mathrm{sn}(u, m)^2\mathrm{sn}(v, m)^2} \quad , \tag{A.20}$$

$$\mathrm{cn}(u + v, m) = \frac{\mathrm{cn}(u, m)\mathrm{cn}(v, m) - \mathrm{sn}(u, m)\mathrm{sn}(v, m)\mathrm{dn}(u, m)\mathrm{dn}(v, m)}{1 - m \cdot \mathrm{sn}(u, m)^2\mathrm{sn}(v, m)^2} \quad \text{and} \tag{A.21}$$

$$\mathrm{dn}(u + v, m) = \frac{\mathrm{dn}(u, m)\mathrm{dn}(v, m) - m \cdot \mathrm{sn}(u, m)\mathrm{sn}(v, m)\mathrm{cn}(u, m)\mathrm{cn}(v, m)}{1 - m \cdot \mathrm{sn}(u, m)^2\mathrm{sn}(v, m)^2} \quad . \tag{A.22}$$

A4 Jacobi Elliptic Functions for $m = 0$ and $m = 1$

As stated above, the parameter m can be thought of as a measure of the eccentricity of the ellipse. The circular case corresponds therefore to the case of $m = 0$. This case implies, that the radius stays constant, and so the dn-function is constant too. The elliptic K reduces to a simple integral

$$K(0) = \int_0^1 \frac{dy}{\sqrt{1 - y^2}} = \frac{\pi}{2} \quad , \tag{A.23}$$

and the elliptic sine and cosine reduce to the well known trigonometric functions. The case of $m = 1$, which corresponds to the case approaching a hyperbola, leads to a divergent elliptic K. This is appropriate, since the hyperbolic functions are not periodic on the real axis. The relations of the elliptic functions, with both the trigonometric and hyperbolic functions are given in table A.4.

$m = 0$	$0 < m < 1$	$m = 1$
$\sin(u)$	$\mathrm{sn}(u, m)$	$\tanh(u)$
$\cos(u)$	$\mathrm{cn}(u, m)$	$\mathrm{sech}(u)$
1	$\mathrm{dn}(u, m)$	$\mathrm{sech}(u)$

TABLE A.4: Elliptic functions for special cases of m-value.

base function	real period	complex period
$\mathrm{sn}(u, m)$	$4K(m)$	$2iK(1-m)$
$\mathrm{cn}(u, m)$	$4K(m)$	$2(K(m) + iK(1-m))$
$\mathrm{dn}(u, m)$	$2K(m)$	$4iK(1-m)$

TABLE A.5: Period and of the base Jacobi elliptic functions in the complex plane.

A5 Generalization

The geometric introduction allows to define the Jacobi elliptic functions in the real axis and to discern very important attributes of them. Nevertheless these functions can be defined in the whole complex plain. The bridge between the already described elliptic functions and the complex Jacobi elliptic functions exceeds the scope of this paper. It can be said however, that these functions are doubly periodic (meaning periodic along two complex axes), and that the periodic properties of the base functions are determined by the complete elliptic integral K, as can be seen in table A.5

APPENDIX B

General Solution of the Lamé Equation

In this section, the solution of the Lamé equation, and its composing special functions, will be examined.

B1 Defining Z, Θ and H with Elliptic Integrals

The relevant elliptic integrals needed to understand the Lamé solution are $\mathbb{E}(u,m)$ and $K(m)$ (for the latter see eq. A.15). The function $\mathbb{E}(u,m)$ is given by

$$\mathbb{E}(u,m) := \int_0^u \mathrm{dn}(u',m)^2 du' \quad , \tag{B.1}$$

the elliptic integral of the second kind. A deeper exploration of $\mathbb{E}(u,m)$ can be found in [WW96], but for the purposes of this work, it suffices to notice, that

$$\mathbb{E}(0,m) = 0 \qquad \text{and} \qquad \frac{d\mathbb{E}(u,m)}{du} = \mathrm{dn}(u,m)^2 \quad . \tag{B.2}$$

Using both $K(m)$, and $\mathbb{E}(u,m)$ it is possible to define the Jacobi Zeta function $Z(u,m)$,

$$Z(u,m) := \mathbb{E}(u,m) - u\frac{\mathbb{E}(K(m),m)}{K(m)} \quad . \tag{B.3}$$

This definition of the Zeta function was introduced, in order *create* a function with the same general properties of $\mathbb{E}(u,m)$, but with a period of $2K(m)$. Therefore, $Z(u,m)$ may be thought of as a normalized $\mathbb{E}(u,m)$, specially regarding its periodic properties.

The Jacobi Theta function $\Theta(u,m)$ can be introduced with the help of $Z(u,m)$ as,

$$\Theta(u,m) := \Theta_0(m) e^{\int_0^u Z(t,m)dt} \quad , \tag{B.4}$$

where Θ_0 is a constant that ranges from zero to one, dependent on the value of m. This value is given by

$$\Theta_0 := \sqrt{\frac{2\sqrt{1-m}K(m)}{\pi}} \tag{B.5}$$

For the definition of the Jacobi Eta function $H(u,m)$ consider the complex generalization of the Theta function $\Theta(u,m)$ inherited from the properties of $\mathrm{dn}(u,k)$ (see tab. A.5).

$$H(u,m) := -i\Theta(u+iK(1-m),m)e^{-\frac{K(1-m)-2iu}{4K(m)}} \quad , \tag{B.6}$$

however, it is important to note, that these functions were originally not defined as above. Jacobi analyzed these functions in his book [Jac29] in 1829, and all the given properties are proved and explained, along with series representations of elliptic functions. Further, the periodicities of $\Theta(u,m)$ and $H(u,m)$ are also derived in this book. They are given by

$$\Theta(u+2K(m),m) = \Theta(u,m) \qquad \text{and} \qquad H(u+2K(m),m) = -H(u,m) \quad , \tag{B.7}$$

respectively.

B2 Solution of the Lamé Equation

The introduction to the special functions in the section above, allow for a qualitative understanding of the solution of the Lamé equation, the general form of which is given by

$$\psi(x)'' = (\ell(\ell+1)m\cdot\mathrm{sn}(x,m)^2 + A)\psi(x) \quad , \tag{B.8}$$

where A is a constant. This equation was studied by Lamé in the 19^{th} century, and its solution can be found in [WW96]. In order to understand the approach behind it, a more thorough treatment of the various forms of the Lamé equation, as well as the elliptic functions is needed, and this goes beyond the scope of the appendix. The solutions are, however, given by

$$\psi(x) = \prod_{r=1}^{\ell} \frac{H(x\pm\tilde{\alpha_r})}{\Theta(x)} e^{\mp xZ(\tilde{\alpha_r})} \quad , \tag{B.9}$$

where the m-dependence is suppressed, and $\tilde{\alpha_1}, \tilde{\alpha_2}, \ldots \tilde{\alpha_\ell}$ are solutions to the following system of equations

$$\begin{cases} \displaystyle\sum_{p=1}^{\ell} \frac{\mathrm{sn}(\tilde{\alpha_p})\mathrm{cn}(\tilde{\alpha_p})\mathrm{dn}(\tilde{\alpha_p}) - \mathrm{sn}(\tilde{\alpha_r})\mathrm{cn}(\tilde{\alpha_r})\mathrm{dn}(\tilde{\alpha_r})}{\mathrm{sn}(\tilde{\alpha_p})^2 - \mathrm{sn}(\tilde{\alpha_r})^2} = 0 \\ \displaystyle\left(\sum_{r=1}^{\ell} \mathrm{cn}(\tilde{\alpha_r})\mathrm{ds}(\tilde{\alpha_r})\right)^2 - \sum_{r=1}^{\ell} \mathrm{ns}(\tilde{\alpha_r})^2 = A \quad . \end{cases} \tag{B.10}$$

Bibliography

[DF98] Gerald Dunne and Joshua Feinberg. 'Self-isospectral periodic potentials and supersymmetric quantum mechanics'. In: *Physical Review D* 57.2 (Jan. 1998), pp. 1271–1276. ISSN: 1089-4918. DOI: 10.1103/physrevd.57.1271. URL: http://dx.doi.org/10.1103/PhysRevD.57.1271.

[GMR17] Asim Gangopadhyaya, Jeffry Mallow and Constantin Rasinariu. *Supersymmetric quantum mechanics: An introduction*. World Scientific Publishing Company, 2017.

[Jac29] Carl Gustav Jacob Jacobi. *Fundamenta nova theoriae functionum ellipticarum. Auctore D. Carolo Gustavo Iacobo Iacobi...* sumtibus fratrum Borntræger, 1829.

[Jaf09] RL Jaffe. *An algebraic approach to reflectionless potentials in one dimension*. 2009.

[Jun12] Georg Junker. *Supersymmetric methods in quantum and statistical physics*. Springer Science & Business Media, 2012.

[Koe08] Erik Koelink. 'Scattering theory'. In: *Lecture Notes, Spring* (2008).

[KS04] Avinash Khare and Uday Sukhatme. 'Periodic potentials and supersymmetry'. In: *Journal of Physics A: Mathematical and General* 37.43 (Oct. 2004), pp. 10037–10055. ISSN: 1361-6447. DOI: 10.1088/0305-4470/37/43/002. URL: http://dx.doi.org/10.1088/0305-4470/37/43/002.

[Kuc12] Peter A Kuchment. *Floquet theory for partial differential equations*. Vol. 60. Birkhäuser, 2012.

[Kuc16] Peter Kuchment. 'An overview of periodic elliptic operators'. In: *Bulletin of the American Mathematical Society* 53.3 (2016), pp. 343–414.

[Mad05] Rafael de la Madrid. 'The role of the rigged Hilbert space in quantum mechanics'. In: *European Journal of Physics* 26.2 (Feb. 2005), pp. 287–312. ISSN: 1361-6404.

DOI: 10.1088/0143-0807/26/2/008. URL: http://dx.doi.org/10.1088/0143-0807/26/2/008.

[MW13] Wilhelm Magnus and Stanley Winkler. *Hill's equation*. Courier Corporation, 2013.

[Nai18] M Thamban Nair. 'Topics in Fourier Analysis-I'. In: (2018).

[OWW10] Adrian Oeftiger, Uwe-Jens Wiese and Urs Wenger. 'Supersymmetric quantum mechanics'. In: *Bachelor Thesis, University of Bern, Switzerland* (2010), pp. 1–38.

[Sch15] William A Schwalm. *Lectures on Selected Topics in Mathematical Physics: Elliptic Functions and Elliptic Integrals*. 2053-2571. Morgan Claypool Publishers, 2015. ISBN: 978-1-6817-4230-4.

[Thi13] Walter Thirring. *Lehrbuch der Mathematischen Physik: Band 3: Quantenmechanik von Atomen und Molekülen*. Vol. 3. Springer-Verlag, 2013.

[Wei05] Steven Weinberg. *The quantum theory of fields: volume 3, supersymmetry*. Cambridge university press, 2005.

[Wip00] Andreas Wipf. 'Introduction to supersymmetry'. In: *Lect. Notes, Uni. Jena, Germany* (2000).

[Wip06] Andreas Wipf. 'Symmetrien in der Physik'. In: *Vorlesungsskript, FSU Jena* (2006).

[WW96] E. T. Whittaker and G. N. Watson. *A Course of Modern Analysis*. 4th ed. Cambridge Mathematical Library. Cambridge University Press, 1996. DOI: 10.1017/CBO9780511608759.