Universiteit Utrecht

Opleiding Natuur- en Sterrenkunde

Applications of integral transformations in mechanical and quantummechanical problems

Bachelor Thesis

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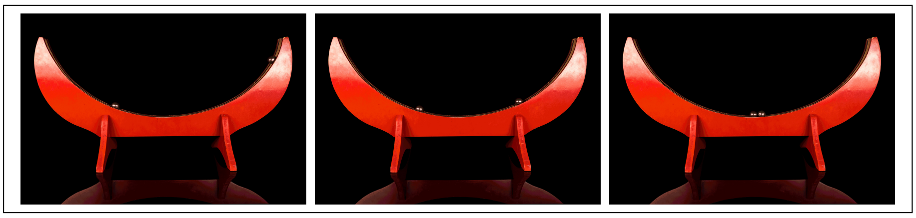

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Abstract

There are many mathematical techniques of which it is unclear how they find their application. We exemplify the diverse application of integral transformations by solving three mechanical and quantummechanical problems in the solution of which integral transformations play a central role. After introducing the general formalism of integral operators we use the Abel operator to determine an exact parametrisation of the isochrone curve. Then we use Fourier transformations to obtain an exact solution for the ground state energy of the one-dimentional Heisenberg model of $E_0/JL = -0.44$, which we compare to a numerical result of $E_0/JL = -0.43$. Lastly we use the Laplace transformation to find the form of the effective Liouvillian L_S^{eff} which acts on the reduced density matrix ρ_S of a single spin-$\frac{1}{2}$ particle coupled to a large reservoir in Laplace space. Lastly, we reflect on these results and conclude that the ability to use integral transformations is essential for any physicist.

The picture on the front page depicts the isochrone curve. On this curve, the time it takes for an object to reach the ground is independent of the height at which it is released. Source: Matemateca (IME/USP), provided via digitalization project by the user: Rodrigo Tetsuo Argenton.

Contents

1 Introduction

In physics courses, much time and effort is attributed to the development and usage of mathematical techniques. One class of techniques that are particularly useful are integral transformations. Not only can the use of these transformations greatly simplify mathematical problems, some problems can only be solved with the use of these transformations. Because of the nature of these transformations, one often has to use the residue theorem to evaluate relevant integrals. The exercises and problems posed in some courses often lack a connection with real research. Therefore we wish to show the reader how useful integral transformations can be by solving real problems in which integral transformations play a crucial role. We will expound three problems, namely the mechanical problem, the determination of the ground state energy of the onedimentional Heisenberg model and lastly, the determination of the form of the reduced density matrix in the single-impurity Kondo model. In order to solve these problems we will respectively make use of three integral transforms, namely the Abel operator, the Fourier transformation and lastly, the Laplace transformation.

In this thesis we shall first present an overview of the abovementioned integral transforms. In the next chapter, we will derive an expression for the mechanical problem using conservation of energy, which we will then solve using the Abel operator. Using this general expression we derive a parametrisation of the isochrone curve. In the chapter after that, we will find an expression for the density of states of the onedimentional Heisenberg model, which we can then find explicitly using the Fourier transformation. With this density of states we then calculate the ground state energy, which we then verify with a numerical diagonalisation of the Hamiltonian. In the chapter following that, we will first get the density matrix of the full single-impurity Kondo model using the Von Neumann equation. After using the Laplace transformation we will find the reduced density matrix in Laplace space. Transforming back to time-space using the inverse Laplace transformation will give us an expression for the reduced density matrix of the spin. In the last chapter we will recapitulate the results and reflect on them. In the appendix we prove some results which are used in the thesis.

2 Integral Transforms

An integral transform is a relation of the form

$$f(x) = \int_a^b g(t)K(x,t)\ \mathrm{d}t, \tag{2.1}$$

where $f(x)$ is the transform of $g(t)$ with respect to the kernel $K(x,t)$ [1, Chapter 15]. Should we write the integral transform as an operator L such that

$$f(x) = Lg(t), \tag{2.2}$$

then L is easily seen to be a linear operator. So we might wonder under which conditions on g, the inverse L^{-1} exists for a kernel K. In this thesis we will be considering three integral transforms: the Fourier transform, the Abel operator and the Laplace transform. Firstly, the Fourier transform $\mathcal{F}$ defined by

$$f(x) = \mathcal{F}[g(t)] = \frac{1}{2\pi}\int_{-\infty}^{\infty} g(t)e^{ixt}\ \mathrm{d}t \tag{2.3}$$

has an inverse $\mathcal{F}^{-1}$ given by

$$g(t) = \mathcal{F}^{-1}[f(x)] = \int_{-\infty}^{\infty} f(x)e^{-ixt}\ \mathrm{d}x \tag{2.4}$$

if f is absolutely integrable and satisfies the *Dirichlet conditions*. That is: f has only a finite number of finite discontinuities, no infinite discontinuities and only a finite number of extrema [4]. Note that there exist some functions on which it is possible to apply the Fourier transformation and its inverse, whilst not satisfying the Dirichlet conditions. These functions are not the within focus of this thesis. Secondly, the Abel operator J^α defined by

$$f(x) = J^\alpha[g(t)] = \int_0^x \frac{(x-t)^{\alpha-1}}{\Gamma(\alpha)} g(t)\ \mathrm{d}t, \tag{2.5}$$

where the Euler-Gamma function for $\alpha > 0$ is given by

$$\Gamma(\alpha) = \int_0^\infty t^{\alpha-1}e^{-t}\ \mathrm{d}t, \tag{2.6}$$

has an inverse $D^\alpha := (J^\alpha)^{-1}$ given by

$$g(t) = D^\alpha[f(x)] = \frac{1}{\Gamma(1-\alpha)}\frac{d}{dt}\int_0^t (t-x)^{-\alpha} f(x)\ \mathrm{d}x \tag{2.7}$$

if f is absolutely continuous [3]. Lastly, the Laplace transform $\mathcal{L}$ defined by

$$f(z) = \mathcal{L}[g(t)] = \int_0^\infty e^{-zt} g(t)\ \mathrm{d}t \tag{2.8}$$

has an inverse $\mathcal{L}^{-1}$ given by

$$g(t) = \mathcal{L}[f(z)] = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{zt} f(z)\ \mathrm{d}z \tag{2.9}$$

with the convergence condition $Re(z) \geq \gamma$. In addition the integrand must satisfy the abovementioned Dirichlet contitions. Equivalently, by substituting $z \to -iz$, and introducing a "starting time" t_0 we may write the transform as follows:

$$f'(z) = f(-iz) = \mathcal{L}[g(t)] = \int_{t_0}^{\infty} e^{iz(t-t_0)} g(t) \, \mathrm{d}t, \tag{2.10}$$

and the inverse $\mathcal{L}^{-1}$ is given by

$$g(t) = \mathcal{L}[f'(iz)] = \frac{-1}{2\pi} \int_{i\gamma-\infty}^{i\gamma+\infty} e^{-iz(t-t_0)} f'(z) \, \mathrm{d}z. \tag{2.11}$$

The convergence condition now becomes $Im(z) \geq \gamma$.

3 Mechanical problem

In this section we follow the book by Gorenflo and Vessella [3]. Consider the following problem: Consider a particle that is subject to gravity g. Let the y be the height in the x, y-plane, and let there be no friction. Let the falling $\tau(y_0)$ be defined as the time it takes the particle to reach the ground ($y = 0$) if it is released from some height y_0. Which curve $x = \phi(y)$ must the particle follow such that it corresponds to a given falling time τ for each starting height y_0?

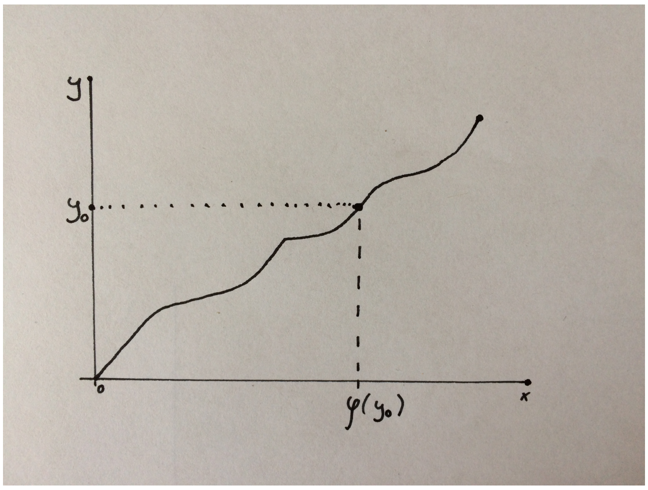

Figure 1: For each starting height y_0 there is a falling time $\tau(y_0)$. If τ is given, what is the curve $\phi(y)$?

The relation between τ and ϕ can by found by using conservation of energy:

$$mg(y_0 - y) = \frac{1}{2} m \mathbf{v}^2, \tag{3.1}$$

$$2g(y_0 - y) = \left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2 = \left(\left(\frac{d\phi}{dy}\right)^2 + 1\right)\left(\frac{dy}{dt}\right)^2, \tag{3.2}$$

such that

$$\sqrt{2g} = \frac{1}{\sqrt{y_0 - y}} \sqrt{1 + \left(\frac{d\phi}{dy}\right)^2} \frac{dy}{dt} \ . \tag{3.3}$$

Integrating, we obtain

(3.4)

$$\tau(y_0) = \frac{1}{\sqrt{2g}} \int_0^{\tau(y_0)} \sqrt{\frac{1 + \phi'(y)^2}{y_0 - y}} \frac{dy}{dt} \ \mathrm{d}t \tag{3.5}$$

$$= \frac{1}{\sqrt{2g}} \int_0^{y_0} \sqrt{\frac{1 + \phi'(y)^2}{y_0 - y}} \ \mathrm{d}y \ . \tag{3.6}$$

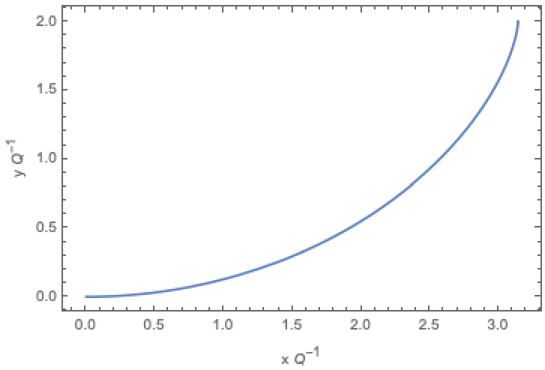

Figure 2: Plot of the isochrone curve. Under constant acceleration g in the downward y direction and without friction, the falling time is equal to c, regardless of the starting height y_0. We denote $Q = \frac{gc^2}{\pi^2}$.

Now we will write this equation in the formalism of the abel operator. Noting that $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$ we can write

$$\tau(y_0) = \sqrt{\frac{\pi}{2g}}\ J^{\frac{1}{2}}\left[\sqrt{1+\phi'(y)^2}\right], \tag{3.7}$$

so, for given $\tau(y_0)$, we obtain the following result:

$$\sqrt{1+\phi'(y)^2} = D^{\frac{1}{2}}\left[\sqrt{\frac{2g}{\pi}}\tau(y_0)\right] \tag{3.8}$$

$$= \frac{\sqrt{2g}}{\pi}\frac{d}{dy}\int_0^y \frac{\tau(y_0)}{\sqrt{y-y_0}}\ \mathrm{d}y_0\ , \tag{3.9}$$

such that

$$1+\phi'(y)^2 = \frac{2g}{\pi^2}\left(\frac{d}{dy}\int_0^y \frac{\tau(x)}{\sqrt{y-x}}\ \mathrm{d}x\right)^2. \tag{3.10}$$

Now we shall use this result to calculate the slope of the *isochrone problem*. The isochrone problem is a well known curve on which the time it takes a particle to reach the ground is always equal to some constant c, regardless of the initial starting height y_0. That is, $\tau(y_0) = c$ for all y_0. So

$$1+\phi'(y)^2 = \frac{2g}{\pi^2}\left(\frac{d}{dy}\int_0^y \frac{c}{\sqrt{y-x}}\ \mathrm{d}x\right)^2 \tag{3.11}$$

$$= \frac{2gc^2}{\pi^2 y}\ . \tag{3.12}$$

This equation is solved by the following parametrisation: [3, p.13]

$$y = \frac{gc^2}{\pi^2}(1-\cos(t)), \tag{3.13}$$

$$x = \frac{gc^2}{\pi^2}(t+\sin(t)). \tag{3.14}$$

Indeed, we can see that

$$\left(\frac{dy}{dt}\right)^2\left[1+\phi'(y)^2\right] = \left(\frac{dy}{dt}\right)^2 + \left(\frac{dx}{dt}\right)^2 = 2\left(\frac{gc^2}{\pi^2}\right)^2(1+\cos(t)) \tag{3.15}$$

$$= 2\left(\frac{gc^2}{\pi^2}\right)^2\frac{\sin^2(t)}{1-\cos(t)} = \left(\frac{dy}{dt}\right)^2\left[\left(\frac{2gc^2}{\pi^2}\right)\frac{1}{y}\right], \tag{3.16}$$

thus solving our differential equation. The isochrone curve is plotted in Figure 2. Since our result is analytical, we will not discuss the vericaty of it. However, some other remarks can be made, which we will make in section 6.

4 Heisenberg Model and Bethe Ansatz

Let us consider a one-dimentional chain of L spin-$\frac{1}{2}$ particles on a lattice with lattice spacing a. The spin of the particle at position j is denoted by $\overrightarrow{S_j} = (S_j^x, S_j^y, S_j^z)$. J is the interaction energy between the spin components in the x and y direction, and ΔJ is the interaction energy between the z-component of the spins. This model is also known as the Heisenberg model. Our goal in this section is to determine the ground state energy E_0 of the model. We will largely follow the book by Thierry Giamarchi [2]. Our result will be determined analytically using an assumption called the Bethe-Ansatz. In particular we will make use of the Fourier transformation to calculate our final result, and we will support this result using a numerical calculation.

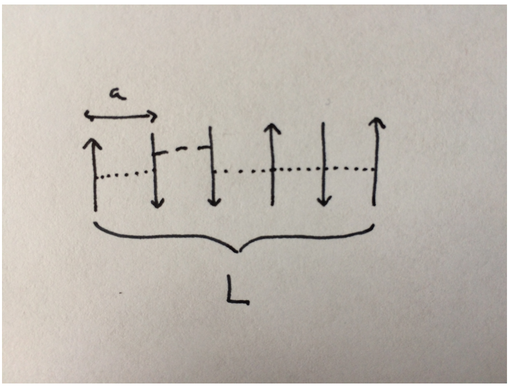

Figure 3: L spins are on a lattice with lattice spacing a. The interaction between adjacent downspins is different from the interaction between alterating spins.

Allowing only for nearest-neighbour interactions we can write the Hamiltonian of the one-dimentional spin chain as

$$\begin{aligned} H &= J \sum_j \left(S_{j+1}^x S_j^x + S_{j+1}^y S_j^y \right) + J\Delta \sum_j \left(S_{j+1}^z S_j^z \right) \\ &= \frac{J}{2} \sum_j \left(S_{j+1}^+ S_j^- + S_{j+1}^- S_j^+ \right) + J\Delta \sum_j \left(S_{j+1}^z S_j^z \right). \end{aligned} \quad (4.1)$$

In the following we will begin in a state with L up spins on a lattice with spacing a=1, and continue with the derivation of the schrödinger equation and corresponding wavefunction for one and two down spins , before using the Bethe Ansatz to generalise our findings to N down spins.

Let's assume periodic boundary conditions throughout this section. In the all up-spin state it is clear from the hamiltonian (4.1) that the energy is equal to $E_0 = \frac{LJ\Delta}{4}$. If we now consider the situation with one down spin, the Schrödinger equation reads

$$E\psi(x) = H\psi(x) = E_0\psi(x) + \frac{J}{2}\big(\psi(x+1) + \psi(x-1)\big) - J\Delta\psi(x), \quad (4.2)$$

in which we recognise that the eigenstates must have the plane wave form

$$\psi(x) = \frac{1}{\sqrt{L}} e^{ikx}. \tag{4.3}$$

Should we now consider the situation with two down spins, we can begin by noting that for large and small distances between particles the energy and momentum must be conserved. We must distinguish between the situation where the spins are either adjacent or not adjacent to each other. This is illustrated in Figure 3. When the spins are not adjacent (... ↓↑↓ ...) the downspins do not feel eachother, and we essentially have the same situation that we considered in the case of one spin down. We can consider two particles in a situation where particle 1 has momentum k_1 and particle 2 has momentum k_2, and compare it to some other situation where the respective momenta of the these particles are k_1' and k_2'. Because the total energy and momentum must be conserved it follows that either $k_1{=}k_1'$ and $k_2{=}k_2'$, or, $k_1{=}k_2'$ and $k_2{=}k_1'$. So when the downspins are *not* adjacent, the wavefunction can be written, for some α and β, as

$$\psi(x_1, x_2) = \alpha e^{i(k_1x_1+k_2x_2)} + \beta e^{i(k_1x_2+k_2x_1)}. \tag{4.4}$$

From periodic boundary conditions, it follows that

$$\psi(x_1, x_2) = \psi(x_2, x_1) = \psi(x_2, x_1 + L), \tag{4.5}$$

$$\alpha = \beta e^{ik_1L} = \beta e^{-ik_2L}. \tag{4.6}$$

When the spins are adjacent, however, (... ↓↓ ...) the situation is different. In this case, the wavefunction must satisfy from the Hamiltonian:

$$(H - E_0)\psi(x, x+1) = \frac{J}{2}\big(\psi(x-1, x+1) + \psi(x, x+2)\big) - J\Delta\psi(x, x+1). \tag{4.7}$$

Here comes in the idea of the Bethe-Ansatz. We want to generalise the wavefunction 4.4 so that it is a solution to the Schrödinger equation, even when the down spins are adjacent. This is only the case if the difference between equations 4.7 and 4.2 is equal to zero:

$$J\Delta\psi(x, x+1) - \frac{J}{2}\big(\psi(x, x) + \psi(x+1, x+1)\big) = 0. \tag{4.8}$$

To accomplish this we may derive that [2, *p. 142*]:

$$\frac{\alpha}{\beta} = -e^{i\Theta(k_1,k_2)}, \tag{4.9}$$

$$\Theta(k_1, k_2) = 2\text{arctan}\left(\frac{\Delta\text{sin}(\frac{k_1-k_2}{2})}{\Delta\text{cos}(\frac{k_1-k_2}{2}) - \cos(\frac{k_1+k_2}{2})}\right). \tag{4.10}$$

Using 4.6 we may conclude that

$$Lk_1 = \pi n + \Theta(k_1, k_2), \tag{4.11}$$

$$Lk_2 = \pi n' + \Theta(k_2, k_1), \tag{4.12}$$

For some integers n, n'.

Should we now consider a system with N down spins, we lose our neat relation 4.6 that we used to derive the previous result. So there is no guarantee that a wavefunction of the form 4.4 will be a solution to the Schrödinger equation. However, if we make an attempt to hold this form we might find a solution anyhow. In the book of Giamarchi [2, *paragraph 5.1.3*] it is derived that, by looking for a wavefunction of the form

$$\psi(x_1, ..., x_N) = \sum_{P \in S_N} A_P e^{\left[i \sum_{j=1}^{N} k_{Pj} x_j\right]}, \tag{4.13}$$

where S_N is the set of all permutations of down spins and A_P is a coefficient corresponding to a permutation P, that the momenta are determined by

$$Lk_i = 2\pi n_i + \sum_j \Theta(k_i, k_j) \tag{4.14}$$

for $n_i \in \mathbb{Z}$ (odd N), or $n_i \in \mathbb{Z} + \frac{1}{2}$ (even N). As such the total energy E and momentum P are given by

$$P = \sum_i k_i, \tag{4.15}$$

$$E = \frac{\Delta J L}{4} + J \sum_j \big(\cos(k_j) - \Delta\big). \tag{4.16}$$

If we consider the situation where $\Delta = 1$ and parametrise k such that

$$\lambda = -\frac{1}{2}\tan(\frac{k - \pi}{2}), \tag{4.17}$$

the equations become

$$2\pi n'_i = 2L\text{arctan}(2\lambda_i) - \sum_j 2\text{arctan}(\lambda_i - \lambda_j), \tag{4.18}$$

$$E = \frac{\Delta |J| L}{4} - |J| \sum_j \frac{2}{1 + 4\lambda_j^2}, \tag{4.19}$$

where $n'_i \in \mathbb{Z}$ (L and N have opposite parities), or $n'_i \in \mathbb{Z} + \frac{1}{2}$ (L and N have equal parities). To find a solution we first need to find the density of states. We define the function $\Phi(\lambda)$ by

$$\Phi(\lambda) = 2L\text{arctan}(2\lambda) - \sum_j 2\text{arctan}(\lambda - \lambda_j). \tag{4.20}$$

In the thermodynamic limit, if we assume that there is no magnetic field, the density of states can be defined as follows (for the argument I refer to [2, p.149]):

$$\rho(\lambda) = \frac{1}{2\pi} \frac{d\Phi}{d\lambda}. \tag{4.21}$$

With this density of states it follows that

$$\Phi(\lambda) = 2L \ \text{arctan}(2\lambda) - 2 \int_{-\infty}^{\infty} \text{d}\lambda' \rho(\lambda') \text{arctan}(\lambda - \lambda'). \tag{4.22}$$

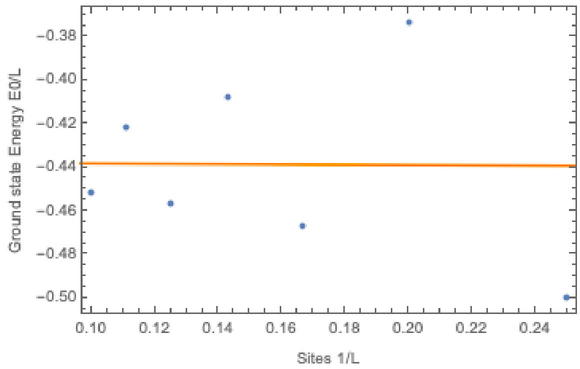

Figure 4: Results of an eigenvalue calculation of the 1D-Heisenberg model simulation in Mathematica. The ground state energy corresponds to the smallest eigenvalue: fitting the results leads to the result $E_0/JL = -0.43$.

Now we shall attempt to obtain an explicit formula for the density of states as a function of λ, such that we may explicitly calculate the energy. In the derivation we will use fourier transformations, denoting the transform of a function $f(x)$ by $\mathcal{F}[f(x)](\omega)$. For the full derivation of some steps we refer to the appendix.

We begin by differentiating 4.22:

$$2\pi\rho(\lambda) = \frac{4L}{1+4\lambda^2} - 2\int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda'\ \rho(\lambda')}{1+(\lambda-\lambda')^2}. \tag{4.23}$$

Next, by applying inverse fourier transformations on the first two terms and using the convolution theorem (A.1) on the third term, we obtain

$$2\pi \int_{-\infty}^{\infty} e^{-i\omega\lambda} \mathcal{F}\big[\rho(\lambda)\big](\omega)\ \mathrm{d}\omega \ = $$
$$\int_{-\infty}^{\infty} e^{-i\omega\lambda} \mathcal{F}\left[\frac{4L}{1+4\lambda^2}\right](\omega)\ \mathrm{d}\omega - 4\pi \int_{-\infty}^{\infty} e^{-i\omega\lambda} \mathcal{F}\big[\rho(\lambda)\big](\omega)\ \mathcal{F}\left[\frac{1}{1+\lambda^2}\right](\omega)\ \mathrm{d}\omega.$$

Now note from (A.3) that

$$\mathcal{F}\left[\frac{1}{1+(ax)^2}\right](\omega) = \frac{e^{-\frac{\omega}{a}}}{2a}, \tag{4.24}$$

so

$$\int_{-\infty}^{\infty} e^{-i\omega\lambda} \left(\mathcal{F}\big[\rho(\lambda)\big](\omega)\ 2\pi(1+e^{-\omega}) - Le^{\frac{-\omega}{2}}\right) \mathrm{d}\omega = 0, \tag{4.25}$$

such that

$$\mathcal{F}\big[\rho(\lambda)\big](\omega) = \frac{L}{2\pi} \frac{e^{\frac{-\omega}{2}}}{1+e^{-\omega}} = \frac{L}{4\pi} \frac{1}{\cosh(\frac{\omega}{2})}. \tag{4.26}$$

Now we conclude from (A.3) that

$$\rho(\lambda) = \int_{-\infty}^{\infty} e^{-i\omega\lambda} \mathcal{F}\big[\rho(\lambda)\big](\omega) \, \mathrm{d}\omega$$
$$= \int_{-\infty}^{\infty} e^{-i\omega\lambda} \, \frac{L}{4\pi} \frac{1}{\cosh(\frac{\omega}{2})} \mathrm{d}\omega = \frac{L}{2\cosh(\pi\lambda)}. \tag{4.27}$$

Now that we have explicitly found the density of states, we can use 4.19 in order to find the ground state energy E_0 (For the derivation, see A.3):

$$E_0 = \frac{L|J|}{4} - |J| \sum_j \frac{2}{1+4\lambda_j^2} \tag{4.28}$$
$$= \frac{L|J|}{4} - |J| \int_{-\infty}^{\infty} \frac{2}{1+4\lambda^2} \, \rho(\lambda) \mathrm{d}\lambda \tag{4.29}$$
$$= \frac{L|J|}{4} - L|J| \log(2) \approx -0.44 L|J|. \tag{4.30}$$

To verify this result, we build the hamiltonian (4.1) in Mathematica and numerically calculate the eigenvalues for different lattice sizes. We then fit linearly over the first ten sites to obtain the result $E_0/LJ = -0.43$, which is in line with the result obtained from the exact Bethe-Ansatz derivation. See Figure 4. We will reflect on this result in section 6.

5 Kondo Model

In this section we will consider a spin-$\frac{1}{2}$ particle that is coupled to a large reservoir (Figure 5), a model that is also known as the *single-impurity Kondo model.* Our goal here is to find an expression for the time evolution of the reduced density matrix ρ_S of the spin. To do this, we will make use of the Laplace transformation.

Following an article of Schuricht and Schoeller [5], we describe the Hamiltonian of the system as the sum of a spin part H_S, a coupling V and a reservoir part H_{res}, such that

$$H = H_S + H_{res} + V. \tag{5.1}$$

The density matrix ρ of the entire system must satisfy the Von Neumann equation

$$\rho(t) = e^{-iH(t-t_0)}\rho(t_0)e^{iH(t-t_0)} = e^{iL(t-t_0)}\rho(t_0), \tag{5.2}$$

where the Liouvillian L is defined by

$$L = [H, .\ ]. \tag{5.3}$$

Thus the Laplace transform $\tilde{\rho}$ of ρ is given by

$$\tilde{\rho}(z) = \int_{t_0}^{\infty} e^{iz(t-t_0)}\rho(t)\ \mathrm{d}t \tag{5.4}$$

$$= \int_{t_0}^{\infty} e^{i(z-L)(t-t_0)}\rho(t_0)\ \mathrm{d}t = \frac{i}{z-L}\rho(t_0), \tag{5.5}$$

by evaluating the integral. Now we can trace out the reservoir part of the density matrix to obtain the transform $\tilde{\rho}_S$ of the reduced density matrix ρ_S of the spin:

$$\tilde{\rho}_S(z) = \mathrm{Tr}_{res}\tilde{\rho}(z) = \frac{i}{z - L_S^{eff}(z)}\rho_S(t_0), \tag{5.6}$$

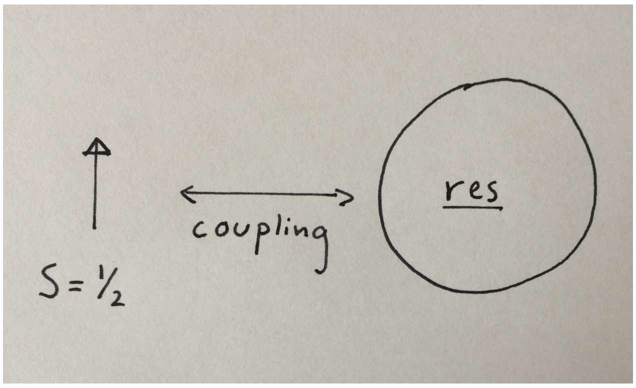

Figure 5: A spin-$\frac{1}{2}$ particle is coupled to a reservoir. The Hamiltonian can be decomposed in a spin part H_S, a coupling V and a reservoir part H_{res}, such that $H = H_S + H_{res} + V$

where $L_S^{eff} = L_S + \Sigma$, the term Σ encoding the contribution of the coupling. L_S^{eff} acts as a linear operator on ρ_S. Since ρ_S is a linear operator on $\mathbb{C}^2$, it has four entries. Thus L_S^{eff} can be written as a 4x4- matrix which acts on $\mathbb{C}^4$. So, if we denote the eigenvectors of L_S^{eff} by $|i\rangle, i \in \{0, 1, -, +\}$, we can write

$$L_S^{eff} = \sum_i c_i |i\rangle\langle i|. \tag{5.7}$$

Because $\sum_i |i\rangle\langle i| = \mathbb{I}_4$, we can write

$$z - L_S^{eff} = \sum_i (z - c_i)|i\rangle\langle i|. \tag{5.8}$$

Using $\langle i|j\rangle = \delta_{i,j}$ we can see immediately that

$$(z - L_S^{eff})^{-1} = \sum_i (z - c_i)^{-1}|i\rangle\langle i|, \tag{5.9}$$

because

$$(z - L_S^{eff})^{-1}(z - L_S^{eff}) = \sum_i \sum_j (z - c_i)^{-1}(z - c_j)|i\rangle\langle i|j\rangle\langle j| \tag{5.10}$$

$$= \sum_i |i\rangle\langle i| = \mathbb{I}_4. \tag{5.11}$$

Using 5.9 and denoting $|i\rangle\langle i| = P_i$, $\tilde{\rho}_S$ can be written as

$$\tilde{\rho}_S(z) = \sum_j \frac{i}{z - c_j} P_j \ \rho_S(t_0). \tag{5.12}$$

Now we can calculate ρ_S using the inverse Laplace transformation, where we let $\gamma \downarrow 0$:

$$\rho_S(t) = \frac{-1}{2\pi} \int_{-\infty+i0^+}^{+\infty+i0^+} e^{-iz(t-t_0)} \tilde{\rho}_S(z) \ \mathrm{d}z \tag{5.13}$$

$$= \frac{1}{2\pi i} \sum_j \int_{-\infty+i0^+}^{+\infty+i0^+} \frac{e^{-iz(t-t_0)}}{z - c_j(z)} P_j(z)\rho_S(t_0) \ \mathrm{d}z \ . \tag{5.14}$$

Since both the eigenvalues c_j and the projectors P_j depend on z, it is not possible to straightforwardly evaluate the integral. Note however, since we expect $P_j(z)$ to behave smoothly, that the discontinuïties z_j of the integrand are given by the solutions to the equations

$$z_j = c_j(z_j). \tag{5.15}$$

Using the expansions

$$P_j(z) = P_j(z_j), \tag{5.16}$$

$$c_j(z) = c_j(z_j) + (z - z_j)\frac{dc_j}{dz}(z_j), \tag{5.17}$$

and noting, where C is some constant and U the lower semicircle of the complex plane, that

$$\left|\int_U \frac{e^{-izt}}{z-z_j} C dz\right| = \lim_{\rho\to\infty}\left|\int_0^{-\pi} \frac{e^{t\rho\sin\theta} e^{-it\rho\cos\theta}}{\rho e^{i\theta} - z_j} C\rho d\theta\right| \tag{5.18}$$

$$\leq \lim_{\rho\to\infty}\int_0^{-\pi} \left|e^{t\rho\sin\theta}\right|\left|C\right| = 0, \tag{5.19}$$

we obtain

$$\rho_S(t) = \frac{1}{2\pi i}\sum_j \int_{-\infty+i0^+}^{+\infty+i0^+} \frac{e^{-iz(t-t_0)}}{(z-z_j)(1-\frac{dc_j}{dz}(z_j))} P_j(z_j)\rho_S(t_0)\ \mathrm{d}z \tag{5.20}$$

$$= \sum_j \frac{e^{-iz_j(t-t_0)}}{(1-\frac{dc_j}{dz}(z_j))} P_j(z_j)\rho_S(t_0). \tag{5.21}$$

by Cauchy's integral formula. We can see that if $Im(z_i) > 0$, we will have a density matrix which increases exponentially over time. This is unphysical. So $Im(z_i) \leq 0$, and we are justified in choosing our contour integral over the lower semicircle of the complex plane. It is proven that there exists a stationary state [6]. Because this state is independent of time, there must be at least one eigenvalue $z_0 = 0$. The density matrix must remain Hermitian regardless of basis choice: this means that e^{-iz_1} must be real, which is only the case if z_1 is imaginary. The diagonal elements must be complex conjugates. In other words, $e^{-iRe(z_2)}$=$e^{iRe(z_3)}$, which is the case if $Re(z_2) = -Re(z_3)$. Summing up, for real $\Gamma_i, h \geq 0$, we can write

$$L_S^{eff} = -i\Gamma_1 P_1 + (h - i\Gamma_+)P_+ + (-h - i\Gamma_+)P_- \ . \tag{5.22}$$

As such we have made use of the Laplace transformation to obtain an expression of the time evolution of the density matrix of the spin, as well as an expression for the effective Liouvillian L_S^{eff} which acts on the density matrix in Laplace-space. In the following section we will discuss these results.

6 Conclusions and discussion

We will present a threefold conclusion and discussion, firstly regarding the mechanical problem, secondly the Heisenberg model, thirdly the Kondo model. Lastly we will reflect briefly on the thesis in general.

In the chapter about the mechanical problem (Chapter 3), we derived the parametrisation for the isochrone curve by exact means:

$$y = \frac{gc^2}{\pi^2}(1 - \cos(t)), \tag{6.1}$$

$$x = \frac{gc^2}{\pi^2}(t + \sin(t)). \tag{6.2}$$

All functions were continuous, so we were justified in using the Abel operator. We made the physical assumption that there was no friction: in further research it could be interesting to look at which types of friction allow for a similar type of derivation and which types of friction will inhibit the problem from being exactly solvable. By building the isochrone curve, it could be experimentally verified that objects released from different heights will meet the bottom of the slope at the same time.

In the chapter about the Heisenberg model (Chapter 4) we used the Bethe Ansatz. Because the resulting wavefunction 4.13 is a solution of the Schrödinger equation, we were justified in the continuation of our calculations using the Bethe-Ansatz assumption. In the derivation of our result, all functions satisfied the Dirichlet conditions and therefore we were justified in using the fourier transformations. Our numerical result $\frac{E_0}{JL} = -0.43$ differed slightly from the exact result $\frac{E_0}{JL} = -0.44$. This difference can be explained by the fact that our numerical simulation only considered small chains up to $L = 10$. By looking at Figure 4 it can be seen that the values converge for larger L, so it is expected that calculations of larger samples will yield a more accurate result. It must be noted that we ommitted the samples for $L \leq 4$, which give unrealistic results because of interfering periodic boundary conditions. Also, we have assumed that only nearest-neighbour interactions are relevant. Therefore it is expected to get better agreement with experiment by including next-nearest-neighbour interactions in the Hamiltonian.

In the chapter about the Kondo model (Chapter 5), we derived that the effective Liouvillian L_S^{eff} acting on the reduced density matrix ρ_S of a spin coupled to a reservoir in Laplace space, has to be of the form

$$L_S^{eff} = -i\Gamma_1 P_1 + (h - i\Gamma_+)P_+ + (-h - i\Gamma_+)P_- \ . \tag{6.3}$$

To obtain this result we used the physical assumptions that the density matrix has to be hermitian and that there exists a stationary state. All integrands satisfied the Dirichlet conditions, so we were justified in using the Laplace transformation. We used Taylor expansions around the poles so that we could apply the inverse Laplace transformation, which is justified because the subsequent contour integration is concerned only with behaviour around the poles. The Kondo model can find applications in, and similarly can be verified in experiment through, for example, the properties of a material which has a single impurity. Also, it has been stated that transport experiments through quantum dots can be verified using the Kondo model, which means it can have applications in nanotechnology [5].

The use of integral transformations was essential to obtain our results. In this thesis we have made clear that integral equations can be used to solve different problems in both quantum and Newtonian mechanics. As such they make up an invaluable instrument which cannot be absent from any physician's toolbox.

Appendix

This appendix consists of proofs of the mathematical techniques used and derivations of relevant results.

A Fourier Transformations

A.1 Convolution Theorem

We will present here a proof of the convolution theorem for fourier transformations. The proof is based on [1, p. 952]. Firstly, we define the fourier transform $\mathcal{F}$ and its inverse $\mathcal{F}^{-1}$ to be

$$\mathcal{F}[g(t)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} g(t) e^{ixt} \ \mathrm{d}t \tag{A.1}$$

$$\mathcal{F}^{-1}[f(x)] = \int_{-\infty}^{\infty} f(x) e^{-ixt} \ \mathrm{d}x \tag{A.2}$$

Now let h be a convolution, that is, we can write

$$h(x) = \int_{-\infty}^{\infty} g(y) f(x-y) \ \mathrm{d}y \tag{A.3}$$

for some f and g. Then

$$\begin{aligned} h(x) &= \int_{-\infty}^{\infty} g(y) f(x-y) \ \mathrm{d}y & \text{(A.4)} \\ &= \int_{-\infty}^{\infty} g(y) \int_{-\infty}^{\infty} \mathcal{F}[f](t) e^{-it(x-y)} \ \mathrm{d}t \ \mathrm{d}y & \text{(A.5)} \\ &= \int_{-\infty}^{\infty} \mathcal{F}[f](t) \left[\int_{-\infty}^{\infty} g(y) e^{ity} \ \mathrm{d}y \right] e^{-itx} \mathrm{d}t & \text{(A.6)} \\ &= 2\pi \int_{-\infty}^{\infty} \mathcal{F}[f](t) \ \mathcal{F}[g](t) \ \mathrm{d}t & \text{(A.7)} \end{aligned}$$

Such that we have obtained the **convolution theorem**:

$$\int_{-\infty}^{\infty} g(y) f(x-y) \ \mathrm{d}y = 2\pi \int_{-\infty}^{\infty} \mathcal{F}[f](t) \ \mathcal{F}[g](t) \ \mathrm{d}t \tag{A.8}$$

A.2 Residue theorem

In this thesis we repeatedly use the **residue theorem**: if f is a holomorphic (that is, locally differentiable) function on the complex plane, and if C is a curve which encloses some poles a_k of f, then

$$\oint_C f(z) \mathrm{d}z = 2\pi i \sum_k \mathrm{Res}_f(a_k) \tag{A.9}$$

The residue $\mathrm{Res}_f(a_k)$ of f at a_k can be found using the following formula:

$$\mathrm{Res}_f(a_k) = \frac{1}{(n-1)!} \lim_{z \to a_k} \frac{d^{n-1}}{dz^{n-1}} (z - a_k)^n f(z) \tag{A.10}$$

where n is the order of the pole a_k.

A.3 Proof of used derivations

This section contains relevant derivations that we reference to in the main part of the thesis.

Derivation 1 *The following equation holds:*

$$\mathcal{F}\left[\frac{1}{1+(ax)^2}\right](\omega) = \frac{e^{-\frac{\omega}{a}}}{2a} \tag{A.11}$$

Proof Let f be given by

$$f(x) = \frac{1}{ia} \frac{e^{i\omega x}}{1 - iax} \tag{A.12}$$

and apply Cauchy's integral formula to obtain

$$\mathcal{F}\left[\frac{1}{1+(ax)^2}\right](\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{f(x)}{x - \frac{i}{a}} \mathrm{d}x = if\left(\frac{i}{a}\right) = \frac{e^{-\frac{\omega}{a}}}{2a} \tag{A.13}$$

Derivation 2 *The following equation holds:*

$$\int_{-\infty}^{\infty} e^{-i\omega\lambda} \frac{L}{4\pi} \frac{1}{\cosh(\frac{\omega}{2})} \mathrm{d}\omega = \frac{L}{2\cosh(\pi\lambda)} \tag{A.14}$$

Proof We will use the residue theorem. Let C be the upper semicircle of the complex plane with radius ρ, then we can immediately see that

$$\left|\left| \int_C f(z)\ \mathrm{d}z \right|\right| = \lim_{\rho \to \infty} \left|\left| \int_0^{\pi} f(\rho, \theta) \rho \mathrm{d}\theta \right|\right| \tag{A.15}$$

$$\leq \lim_{\rho \to \infty} \int_0^{\pi} \left|\left| \frac{L}{4\pi} \frac{\rho}{1+\rho^2} \mathrm{d}\theta \right|\right| = 0 \tag{A.16}$$

The poles of f are given by

$$a_k = 2\pi i \left(k + \frac{1}{2}\right) \tag{A.17}$$

Now, by the residue theorem,

$$\oint f(z) \mathrm{d}z = \int_{-\infty}^{\infty} f(\omega) \mathrm{d}\omega + \oint_C f(z)\ dz = 2\pi i \sum_{k=0}^{\infty} \mathrm{Res}_f(a_k) \tag{A.18}$$

Observe that

$$\begin{aligned}
\text{Res}_f(a_k) &= \lim_{z\to a_k}(z-a_k)f(z) && \text{(A.19)}\\
&= \frac{L}{4\pi}\lim_{z\to a_k}\frac{(z-a_k)e^{iz\lambda}}{\cosh(\frac{z}{2})} && \text{(A.20)}\\
&= \frac{L}{4\pi}\lim_{y\to 0}\frac{ye^{i\lambda(y+a_k)}}{(-1)^k\ i\ \sinh(\frac{y}{2})} && \text{(A.21)}\\
&= \frac{(-1)^k L}{4\pi i}e^{ia_k\lambda}\lim_{y\to 0}\frac{y}{\frac{y}{2}+\mathcal{O}(y^3)} = \frac{(-1)^k L}{2\pi i}e^{ia_k\lambda} && \text{(A.22)}
\end{aligned}$$

such that

$$\begin{aligned}
2\pi i\sum_{k=0}^{\infty}\text{Res}_f(a_k) &= Le^{-\pi\lambda}\sum_{k=0}^{\infty}e^{-2\pi k\lambda}(-1)^k && \text{(A.23)}\\
&= Le^{-\pi\lambda}\sum_{k=0}^{\infty}\big(-e^{-2\pi\lambda}\big)^k && \text{(A.24)}\\
&= \frac{Le^{-\pi\lambda}}{1+e^{-2\pi\lambda}} = \frac{L}{2\cosh(\pi\lambda)} && \text{(A.25)}
\end{aligned}$$

Derivation 3 *The following equation holds:*

$$\int_{-\infty}^{\infty}\frac{1}{1+4\lambda^2}\ \frac{1}{\cosh(\pi\lambda)}\ \mathrm{d}\lambda = \log(2) \tag{A.26}$$

Proof Denote the integrand by f, let C be the upper semicircle of the complex plane with radius ρ, and begin by noting that

$$\begin{aligned}
\left|\left|\int_C f(z)\ \mathrm{d}z\right|\right| &= \lim_{\rho\to\infty}\left|\left|\int_0^{\pi} f(\rho,\theta)\rho\mathrm{d}\theta\ \right|\right| && \text{(A.27)}\\
&\le \lim_{\rho\to\infty}\int_0^{\pi}\left|\left|\frac{1}{1+4\rho^2}\,\frac{\rho}{1+\rho^2}\mathrm{d}\theta\ \right|\right| = 0 && \text{(A.28)}
\end{aligned}$$

note that the poles of f are given by

$$a_k = i\left(k+\frac{1}{2}\right) \tag{A.29}$$

where the poles a_0 and a_{-1} are second order poles, and all the other poles are of the first order. So from the residue theorem,

$$\oint f(z)\mathrm{d}z = \int_{-\infty}^{\infty} f(\lambda)\mathrm{d}\lambda + \int_C f(z)\ dz = 2\pi i\sum_{k=0}^{\infty}\text{Res}_f(a_k) \tag{A.30}$$

First we calculate the residue of the second order pole $a_0 = \frac{i}{2}$, using the substitution $y = z - \frac{i}{2}$, before using the taylorseries of tanh and sinh to obtain the result.

$$\text{Res}_f(a_0) = \lim_{z\to\frac{i}{2}} \left[\frac{d}{dz}(z-\frac{i}{2})^2 f(z)\right] \tag{A.31}$$

$$= \lim_{z\to\frac{i}{2}} \left[\frac{i-\pi(z^2+\frac{1}{4})\ \tanh(\pi z)}{4(z+\frac{i}{2})^2\ \cosh(\pi z)}\right] \tag{A.32}$$

$$= \lim_{y\to 0} \left[\frac{i-\pi y(y+i)\ (\tanh(\pi y))^{-1}}{4i(y+i)^2\ \sinh(\pi y)}\right] \tag{A.33}$$

$$= \lim_{y\to 0} \left[\frac{i-\pi y(y+i)\frac{1+\mathcal{O}(y^2)}{\pi y+\mathcal{O}(y^3)}}{4i(y+i)^2[\pi y+\mathcal{O}(y^3)]}\right] \tag{A.34}$$

$$= \lim_{y\to 0} \frac{-y+i-i\lim_{y\to 0}\frac{\pi y+\mathcal{O}(y^3)}{\pi y+\mathcal{O}(y^3)}}{4i(y+i)^2\pi y} = \frac{1}{4\pi i} \tag{A.35}$$

Then we calculate the residue of any other pole $a_{k>0} = i(k+\frac{1}{2})$. Because the pole is of the first order, it follows, again substituting $y = z - a_k$, that

$$\text{Res}_f(a_k) = \lim_{z\to a_k}(z-a_k)f(z) \tag{A.36}$$

$$= \lim_{z\to a_k} \frac{1}{1+4z^2}\ \frac{z-i(k+\frac{1}{2})}{\cosh(\pi z)} \tag{A.37}$$

$$= \frac{-1}{4k(k+1)} \lim_{y\to 0} \frac{y}{(-1)^k\ i\ \sinh(\pi y)} \tag{A.38}$$

$$= \frac{i(-1)^k}{4k(k+1)} \lim_{y\to 0} \frac{y}{\pi y+\mathcal{O}(y^3)} = \frac{1}{4\pi i}\frac{(-1)^{(k+1)}}{k(k+1)} \tag{A.39}$$

We obtain the result if we sum over all residues:

$$\frac{1}{2\pi i}\oint f(z)\ dz = \sum_{k=0}^{\infty}\text{Res}_f(a_k) \tag{A.40}$$

$$= \frac{1}{4\pi i}\left(1+\sum_{k=1}^{\infty}\frac{(-1)^{(k+1)}}{k(k+1)}\right) \tag{A.41}$$

$$= \frac{1}{2\pi i}\ \log(2) \tag{A.42}$$

Which proves our result.

Appendix B - Simulation Code

```
hbar = 1;
Sx = hbar/2 {{0., 1.}, {1., 0.}};
Sy = hbar/2 {{0., -i}, {i, 0.}};
Sz = hbar/2 {{1., 0.}, {0., -1.}}(*Pauli Matrices*);
Δ = 1.;
J = 1.;

EigL[length_] := Module[{L = length, Sxj, Syj, Szj, H},
  Sxj = Table[KroneckerProduct[IdentityMatrix[2^(j-1)], Sx, IdentityMatrix[2^(L-j)]], {j, L}];
  Syj = Table[KroneckerProduct[IdentityMatrix[2^(j-1)], Sy, IdentityMatrix[2^(L-j)]], {j, L}];
  Szj = Table[KroneckerProduct[IdentityMatrix[2^(j-1)], Sz, IdentityMatrix[2^(L-j)]], {j, L}];
  H = J Sum[Sxj[[Mod[j+1, L, 1]]].Sxj[[j]] + Syj[[Mod[j+1, L, 1]]].Syj[[j]] + Δ*Szj[[Mod[j+1, L, 1]]].Szj[[j]],
     {j, L}];
  Return[Min[Eigenvalues[H]] // N]]

Eiglist = Table[{1/j, EigL[j]/j}, {j, 4, 10}];


nlm = NonlinearModelFit[Eiglist, b x + c, {b, c}, x, Weights → 1/Transpose[Eiglist][[1]]^2]
FittedModel[ -0.437614 - 0.00667838 x ]

pl = Plot[nlm[x], {x, 0, 8}, PlotStyle → Orange];
lp = ListPlot[Eiglist, PlotRange → All];
Show[lp, pl, Frame → True, FrameLabel → {"Sites 1/L", "Ground state Energy E0/L"}]
```

Figure 6: Mathematica code used to simulate the 1D Heisenberg model. The resulting plot can be seen in Figure 4

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