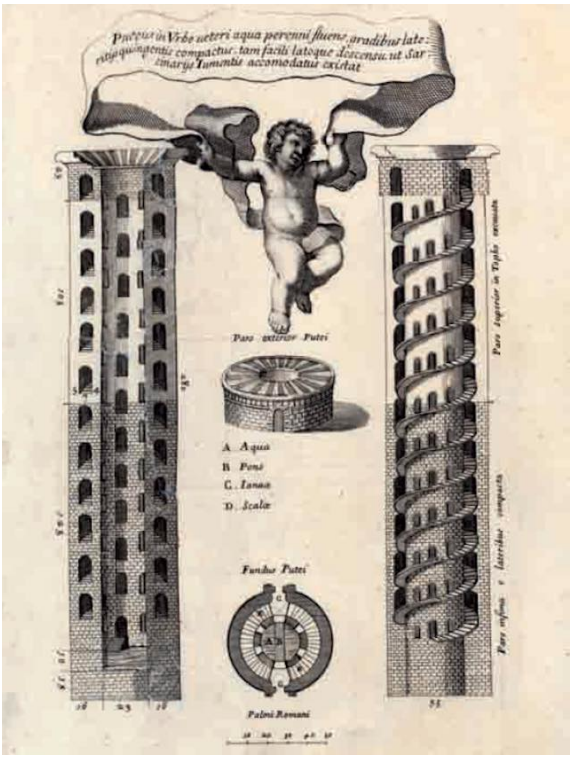
Properties of Quantum Spin Systems and their Classical Limit

From the Quantum Curie-Weiss Model to the Double Well Potential

Master thesis in Mathematical Physics

Radboud University Nijmegen



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Abstract

Let h_N^{CW} be the N-dependent quantum Curie-Weiss spin-1/2 Hamiltonian defined on the Hilbert space $\mathcal{H}_N = \bigotimes_{n=1}^{N} \mathbb{C}$. Since $\mathcal{H}_N$ is finite-dimensional, this Hamiltonian is a bounded operator. Consider then the $\hbar$-dependent unbounded Schrödinger operator with a symmetric double well potential, denoted by $h_\hbar$, and defined on $L^2([0,1])$. We show that both operators are related, in that the quantum Curie-Weiss Hamiltonian can be seen as a discretization of this Schrödinger operator under the identification $N = 1/\hbar$. Moreover, we show that the algebraic (unique) ground state of h_N^{CW} converges to a doubly degenerate classical state on $C(B^3)$ as $N \to \infty$, where $C(B^3)$ is the commutative C^*-algebra of continuous functions on the closed unit ball $B^3 \subset \mathbb{R}^3$. This involves a so-called deformation quantization of $C(B^3)$. We describe how the natural phenomenon of spontaneous symmetry breaking (SSB), that does only play a role in the limit, can already be detected for finite, but large N. Thereto, perturbation theory is used.

Preface

This thesis is an outcome of my final master project written in the last year of my two-year master in Mathematics, with specialization track Mathematical Physics, at the Radboud University Nijmegen. The subject of this thesis was inspired by the Schrödinger operator describing a particle in a symmetric double well. Its quantum-mechanical properties including the classical limit and the phenomenon of spontaneous symmetry breaking are well understood. These facts are less well understood for quantum spin systems. In this thesis we took the quantum spin system called the Curie-Weiss model as our main example. The aim of this project is to analyze this model and its classical limit, and to understand how it can be related to a Schrödinger operator with a symmetric double well potential. In particular, we will see how spontaneous and also explicit symmetry breaking plays a role and how the model is related to the Schrödinger operator. Moreover, we will discuss how the algebraic ground state of this spin Hamiltonian converges to some doubly degenerate classical state (i.e., a function on a commutative C^*-algebra). This involves a deformation quantization map.

First of all, I would like to express my gratitude to professor Klaas Landsman for the supervision of my thesis, his helpful comments and insightful conversations we have had. Moreover, I want to thank you for your support and advice you gave me during my whole study of Mathematics. Having a bachelor degree in Chemistry, it was not easy to study mathematics, but you were always very helpful and emphatic. I would also like to thank professor Gerrit Groenenboom for being the second reader and for his ideas on how to link the quantum spin system to a Schrödinger operator. Moreover, I appreciate his time for answering numerous questions and giving suggestions about numerical computations in MATLAB. Furthermore, I express my gratitude to Robin Reuvers for his help in working out the details regarding the connection with the spin system and this Schrödinger operator. I would like to thank professor Alessandro Michelangeli for arranging my internship in the SISSA Institute, for his useful comments on my work, and for taking the time to discuss it with me, even while he was extremely busy at that moment. I want to thank Luuk Verhoeven for his collaboration on the course in Spontaneous Symmetry Breaking, which was useful for this thesis. Last but not least, I would like to thank my mother for the support she always gives me.

Contents

Chapter 1

Introduction

1.1 Asymptotic emergence

Inspired by the book *Foundations of Quantum Theory* written by Landsman, I decided to immerse myself into the area of higher-level theories H which are limiting cases of lower-level theories L. For example, H is classical mechanics of a particle on the real line with phase space $\mathbb{R}^2 = \{(p, q)\}$ and ensuing C^*-algebra of observables given by $A_0 = C_0(\mathbb{R}^2)$. Then L is quantum mechanics, with a C^*-algebra $A_\hbar$ $(\hbar > 0)$ taken to be the compact operators $B_0(L^2(\mathbb{R}))$ on the Hilbert space $L^2(\mathbb{R})$. Another example is the relation between statistical mechanics of finite quantum and infinite quantum spin systems. Thus H is statistical mechanics of an infinite quantum spin system, given by the quasi-local algebra being the infinite (projective) tensor product of $B = M_n(\mathbb{C})$ with itself, and L is the N-fold (projective) tensor product of B with itself. The last example we give is the one we use in this thesis. In this case H describes classical mechanics on the commutative C^*-algebra $C(B^3)$, with $B^3 \subset \mathbb{R}^3$ the closed unit ball, and L is given by the N-fold tensor product of $M_2(\mathbb{C})$ with itself, and hence describes statistical mechanics of finite quantum spin systems. The limiting relationship between the two theories will be described by a continuous bundle of C^*-algebras. These theories all have in common that the limiting theory H has features that at first sight cannot be explained by the lower-level theory L, because apparently L lacks a property inducing those features in the limit to H. This is what we call *asymptotic emergence*, first introduced in [1], and reformulated in terms of C^*-algebras in [22].

In this thesis we will focus on the natural phenomenon of spontaneous symmetry breaking (SSB). We will see that this is an *emergent* feature of H, since it does not occur in L. This is well known for the example with H being classical mechanics on $C_0(\mathbb{R}^2)$, and L quantum mechanics, where the quantum system is described by Schrödinger operator with a symmetric double well potential. We will see that this phenomenon is also an emergent feature for the pair (H, L), with H describing classical mechanics on $C(B^3)$, and L a finite quantum spin system of spin up and spin down particles. We make a link between the quantum Curie-Weiss model and this Schrödinger operator and argue that, perhaps surprisingly, SSB is indeed compatible with both theories.

1.2 Classical Limit

The theory of quantum mechanics gives a description of systems containing tiny particles. However, in principle it can also be applied to any physical system, in particular to systems of large objects. We know from experience that if we apply a quantum-mechanical theory to such objects, the outcome will be a classical state, which should be describable in the classical limit of quantum mechanics. For example, consider the following Schrödinger equation for a particle with mass m in

a potential well V:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + m_V\psi = \epsilon\psi. \tag{1.1}$$

If we apply this equation to a particle with large mass, then according to the above, it should reproduce classical mechanics. This can equivalently be achieved by letting $\hbar \to 0$ for fixed m. At first sight, this seems strange, as $\hbar$ is a constant. However, many quantum systems can be linked to a classical system by taking the limit $\hbar \to 0$. Such a classical system is well understood in most of the cases, and therefore it is important to understand this limit. We will often refer to this classical limit as $\hbar \to 0$ or $N \to \infty$, depending on the quantum system we consider. We will see that the notion of a continuous bundle of C^*-algebras and a deformation quantization play an important role in understanding and computing this limit.

1.3 Schrödinger operator with a symmetric double well potential

My motivation for studying properties of quantum spin systems is originally based on the Schrödinger operator describing a particle in a symmetric double well potential. This $\hbar$-dependent operator is given by $h_\hbar = -\hbar^2\frac{d^2}{dx^2} + V(x)$, with V a symmetric double well function acting as a multiplication operator. This Hamiltonian has been extensively applied in many branches of physics and theoretical chemistry. For example, it has been used to study quantum tunneling of the nitrogen atom in the ammonia molecule as in [4]. It has been also applied in studies to the mean-field dynamics of Bose-Einstein condensates [35]. Moreover, time-independent behaviour of the double well potential in the classical limit $\hbar \to 0$ has been studied [34]. This will be important when comparing the ground states of the N-dependent quantum Curie-Weiss model to those of the Schrödinger operator with symmetric double well in the semi- classical limit (i.e., N large, but finite) with $N = 1/\hbar$. We shall see that the quantum Curie-Weiss model can be seen as a discretization of this Schrödinger operator.

1.4 The aim of this project

Initially, the goal of this thesis was to understand spontaneous symmetry breaking in some class of quantum spin systems. Based on the symmetric double well potential that is quite well understood, we wanted to give an analog of SSB for spin system models. As explained above, we need two theories describing these spin systems: the higher-level theory H as a limiting case of a lower-level theory L. For example the higher-level theory at $N = \infty$ for the quantum Ising model is described on the quasi-local algebra, whereas for the Curie-Weiss model this algebra is given by the classical commutative C^*-algebra $C(B^3)$, even though the lower-level theories are both described by the same C^*-algebras $B(\mathcal{H}_{\Lambda_N})$, with $\mathcal{H}_{\Lambda_N} = \bigotimes_{n=1}^{N}\mathbb{C}^2$. The reason for this lies in the fact that the quantum Ising Hamiltonian is a short-range model, whereas the Curie-Weiss Hamiltonian falls in the class of homogeneous mean-field models and hence is long range. A very interesting result is that there exists also a second higher-level limit for the quantum Ising model, but this time it is associated with the classical C^*-algebra $C(S^2_{1/2})$, with $S^2_{1/2} \subset \mathbb{R}^3$ the 2-sphere with radius 1/2. One can show that its ground state, modulo a constant, is precisely the ground state for the classical limit of the Curie-Weiss Hamiltonian, which in both cases is doubly degenerate and displays SSB, but for finite N i.e., the lower-level theory, it does not display SSB. This is surprising, because both models fall in different categories. Another question that one can ask oneself is how to construct the classical Hamiltonian on $S^2_{1/2}$ corresponding to the classical limit theory H of the underlying lower-level theory L describing the quantum Ising model for finite N. A similar question can be asked for the quantum Curie-Weiss Hamiltonian, where in this case the classical Hamiltonian is a continuous function given on $C(B^3)$. Since the ground states of both (classical) limiting theories

are the same modulo a constant, one might expect that there is a link between both models, even though they fall in different categories (i.e., long range and short range). The same question can be asked for the ground states of the infinite quantum Ising model and the classical quantum Ising model. Both different limiting models have a doubly degenerate ground state that displays SSB, but the first one is defined on a highly non-commutative C^*-algebra, whereas the latter one is defined on a commutative C^*-algebra. This double degeneracy is also present in the limiting case ($\hbar \to 0$) of the quantum harmonic oscillator, with limit algebra given by the commutative C^*-algebra $C_0(\mathbb{R}^2)$. These topics are therefore worth studying further and in connection with one another. We give a short overview of the relevant quantum operators and their classical analogs:

$$h_N^{\mathrm{CW}} = -\frac{J}{2|\Lambda_N|} \sum_{x,y \in \Lambda_N} \sigma_3(x)\sigma_3(y) - B \sum_{x \in \Lambda} \sigma_1(x) \quad \text{(quantum Curie-Weiss model)} \tag{1.2}$$

$$h_N^{\mathrm{Ising}} = -\sum_{x \in \Lambda_N} (\sigma_3(x)\sigma_3(x+1) + B\sigma_1(x)) \quad \text{(quantum Ising model)} \tag{1.3}$$

$$h_\hbar = -\hbar^2 \frac{d^2}{dx^2} + V(x) \quad \text{(quantum harmonic oscillator with double well potential.)} \tag{1.4}$$

Here Λ_N denotes a finite subset of $\mathbb{Z}$ consisting of N elements. Their classical analogs are in all three cases continuous functions on some commutative C^*-algebra, keeping in mind that the Ising model has also a quantum analog on the quasi-local algebra. These analogs are given below.

$$h_\infty^{\mathrm{CW}}(x,y,z) = -\frac{1}{2}z^2 - Bx \quad \text{(classical Curie-Weiss model)} \tag{1.5}$$

$$h_\infty^{\mathrm{Ising}}(\theta) = -(\frac{1}{2}\cos^2(\theta) + B\sin(\theta)) \quad \text{(classical Ising model)} \tag{1.6}$$

$$h_0(p,q) = p^2 + V(q) \quad \text{(classical harmonic oscillator with double well potential.)} \tag{1.7}$$

As we have mentioned in all the cases above, using a deformation quantization map, one can show that the algebraic ground state of the quantum Hamiltonian does not display SSB and converges to a ground state of the corresponding classical function that does display SSB[1]. These actual ground states states that show SSB are obtained by minimizing the above functions and are therefore given by points in phase space and hence correspond to Dirac measures. The mystery to be resolved is therefore how the classical ground states with SSB arise from the quantum ground states without SSB.

In this project, we will concentrate on the quantum Curie-Weiss model and the quantum harmonic oscillator in a symmetric double well potential with corresponding classical limits, and try to give an insight of their properties and the way they are related. In particular, convergence of the ground state will be discussed as well as the phenomenon of spontaneous symmetry breaking.

1.5 Outline of the thesis

The next (second) chapter discusses the notion of a ground state of a C^*-dynamical system, denoted by the tuple (A, α). Here A denotes a C^*-algebra that plays the role of a physical system and consists of observables quantities to be interpreted as (unbounded) self-adjoint operators on some Hilbert space. The dynamics is given by a (continuous) homomorphism $\alpha : \mathbb{R} \to \mathrm{Aut}(A)$, being the time evolution of the system that describes how observables evolve over time (Heisenberg picture). We will link this general notion of a ground state to the one used in linear algebra, namely the eigenvector(s) corresponding to the lowest eigenvalue. We show that the first general concept

[1]This does not hold for the eigenvectors or eigenfunctions themselves: they fail to converge on the limit algebra, when $N \to \infty$ or $\hbar \to 0$.

extends the one used in Linear Algebra. We then give the definition of spontaneous symmetry breaking (SSB) and show that the quantum Schrödinger operator $h_\hbar$ ($\hbar > 0$) describing a particle in a symmetric double well does *not* display SSB, whereas its classical analog (viz. (1.7)) does.

In Chapter 3 we will state the quantum mechanical Curie-Weiss model ($N < \infty$), being an operator on a 2^N-dimensional Hilbert space. We argue that for each finite N, this operator does not display SSB. The prove of this follows from the uniqueness of the ground state (Chapter 5) and a commutation relation with a unitary operator implementing the symmetry.
We show that the ground state must lie in the range of the symmetrizer operator, so that we may diagonalize this operator with respect to a basis for this range, which is $(N+1)$-dimensional. We show that in the canonical symmetric basis for $\mathrm{ran}(S)$, the quantum Curie-Weiss operator becomes a tridiagonal matrix of dimension $N+1$, and is therefore relative easy to diagonalize with a computer, compared to the one originally defined on the space $\bigotimes_{n=1}^{N} \mathbb{C}^2 \cong \mathbb{C}^{2^N}$.

Then in Chapter 4, we are going to make a link between the Curie-Weiss Hamiltonian, restricted to $\mathrm{ran}(S)$ and scaled by a factor $1/N$, and a Schrödinger operator with a symmetric double well potential, depending on $\hbar = 1/N$. We will see that in some approximation, this scaled compressed Curie-Weiss Hamiltonian corresponds to a matrix representing a discretization of this Schrödinger operator. This discretization gets better when N increases, but N has to be finite in order to speak about a quantum system. Even though in the limit $N \to \infty$ the Schrödinger operator is not well-defined, the ground state eigenfunction still converges to some points minimizing the classical Hamiltonian (1.7). These points in turn correspond to some Dirac measure on the commutative C^*-algebra $C_0([0,1] \times \mathbb{R})$. This involves the notion of a deformation quantization.

Uniqueness of the ground state of the Schrödinger operator $h_\hbar$ ($\hbar > 0$) is achieved when the potential satisfies some properties. The proof is based on an infinite-dimensonal version of the Perron-Frobenous Theorem applied to $e^{-th_\hbar}$ for $t > 0$. In Chapter 5, we state this theorem and theorems and lemmas related, and prove them for the Hilbert space $L^2(\mathbb{R}^n)$. We discuss the Perron-Frobenius theorem for non-negative irreducible matrices and see how this theorem is a specific example of another more general theorem using unbounded operators on a σ-finite measure space. The latter one will be applied to our (compressed) Curie-Weiss matrix in order to prove uniqueness of the ground state.

In Chapter 6, we explain the notion of deformation quantization applied to the quantum Curie-Weiss model. We define such a map and show that the ground state of this quantum system converges indeed to twofold degenerate Dirac measures on the algebra $C(B^3)$, even though the limit of h_N^{CW} as $N \to \infty$ does not exists. These measures correspond to points in B^3 that are the minima of the classical function h_0^{CW}, given by (1.5). Moreover, we will introduce the notion of reduced density matrices and show that the above convergence is an example of taking some limit of such matrices. Partially based on numerics, we prove that we have weak$^*-$ convergence (See §6.2 for details). The last part of this section introduces the Lipkin-Meshkov-Glick (LMG) model, which can be seen as a generalization of the Curie-Weiss model.

Chapter 7 discusses a perturbation in the Curie-Weiss Hamiltonian. We make again the link with the Schrödinger operator describing a particle in a symmetric double well. We show that this perturbation is completely analogous to the asymmetric 'flea' on the double well potential studied in [34]. We argue that, due to the position of this flea, the ground state will localize in one of the wells and therefore will converge to a pure state in the classical limit. This is in contrast with the unperturbed Hamiltonian, where the ground state will a priori converge to a mixed classical state.

The final chapter provides an outlook stating some open problems and some suggestions for further research.

Chapter 2

Ground states and Spontaneous Symmetry Breaking

In this section we study the concept of spontaneous symmetry breaking (SSB). For this, we need an abstract mathematical framework to compute the right limits (see Chapter 6). We start with the notion of a ground state of a C^*-dynamical system. We show that this notion is compatible with the one used in linear algebra, namely eigenvector(s) corresponding to the lowest eigenenergy. Then, we give an example of a higher-level theory H describing classical mechanics on $C_0(\mathbb{R}^2)$, seen as a limiting case of a lower-level theory L describing a quantum system given by a Schrödinger operator with a double well potential. We give a detailed proof that SSB does not occur in L, but does occur in H.

2.1 General setting

The dynamics describes how observables evolve over time, so it says something about the underlying physical system. Such a physical system is mathematically identified with a C^*-algebra A. The dynamics is then given by a continuous[1] homomorpihsm $\alpha : \mathbb{R} \to \mathrm{Aut}(A)$, $t \mapsto \alpha_t$, where we use the notation $\alpha_t \equiv \alpha(t)$. This map is also called the time evolution of the system. In the case that $A = B(H)$, we always have $\alpha_t(a) = u_t a u_t^*$ for some family of unitaries $u_t \equiv u(t)$, $(t \in \mathbb{R})$ (see Appendix A for more details). A C^*-algebra A with dynamics α is called a C^* *dynamical system*, denoted by (A, α). We give the definition of the ground state of a C^*- dynamical system. This definition can be found in [5, sec. 5.3.3 and 6.2.7] or [22, p.350].

Definition 2.1. *Let A be a C^*-algebra with time evolution, i.e., a continuous homomorphism $\alpha : \mathbb{R} \to Aut(A)$. A ground state of (A, α) is a state ω on A such that:*

1. ω is time independent, i.e., $\omega(\alpha_t(a)) = \omega(a)\ \forall a \in A\ \forall t \in \mathbb{R}$.
2. The generator h_ω of the ensuing continuous unitary representation

$$t \mapsto u_t = e^{ith_\omega} \tag{2.1}$$

of $\mathbb{R}$ on $\mathcal{H}_\omega$ has positive spectrum, i.e., $\sigma(h_\omega) \subset \mathbb{R}_+$, or equivalently $\langle \psi, h_\omega \psi \rangle \geqslant 0$ $(\psi \in D(h_\omega))$.

We will give some comments to this definition below and explain where this Hamiltonian is coming from.

We are given a C^*-dynamical system (A, α) and a ground state ω for this system. We can apply the GNS-construction to A and ω (see Appendix A) to obtain a unique triple $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$,

[1] The continuity is explained in Appendix A.

where $\pi_\omega : A \to B(\mathcal{H}_\omega)$ is the GNS-representation of A, $\mathcal{H}_\omega$ is a Hilbert space, and Ω_ω is a cyclic vector for π_ω. In addition, for all $a \in A$ we have

$$\omega(a) = \langle \Omega_\omega, \pi_\omega(a)\Omega_\omega \rangle. \tag{2.2}$$

Now, since by part 1 of Definition 2.1 for each $t \in \mathbb{R}$, the automorphism α_t satisfies $\omega \circ \alpha_t = \omega$, we can apply Theorem A.10 to obtain a family of unitaries $\{u_{\omega,t}\}_t$ such that

$$\pi_\omega(\alpha_t(a)) = u_{\omega,t}\pi_\omega(a)u^*_{\omega,t} \tag{2.3}$$

and

$$u_{\omega,t}\Omega_\omega = \Omega_\omega, \tag{2.4}$$

where, u_t is defined as

$$u_{\omega,t}\pi_\omega(a)\Omega_\omega = \pi_\omega(\alpha_t(a))\Omega_\omega. \tag{2.5}$$

The map $u_{\omega,t}$ is well-defined as follows from the proof of Theorem A.10. This is a general statement in the theory of operator algebras. The next lemma states an important result about this family of unitaries:

Lemma 2.2. *The family $\{u_{\omega,t}\}_t$ of unitaries forms a continuous unitary representation of $\mathbb{R}$ on $\mathcal{H}_\omega$.*

Proof. Since $\alpha : \mathbb{R} \mapsto \mathrm{Aut}(A)$ is a continuous homomorphism, the map $t \to \alpha_t$ is strongly continuous, in that for each $a \in A$, the map $t \mapsto \alpha_t(a)$ is continuous.

We have to show that the map

$$\mathbb{R} \times \mathcal{H}_\omega \to \mathcal{H}_\omega \tag{2.6}$$
$$(t, \psi) \mapsto u_{\omega,t}\psi \tag{2.7}$$

is continuous. It suffices to show this for the dense subspace $H_\omega = \pi_\omega(A)\Omega_\omega$ of $\mathcal{H}_\omega$.
Then, given $\psi, \psi' \in H_\omega$ and $t, t' \in \mathbb{R}$. Consider the norm difference

$$||u_{\omega,t}\psi - u_{\omega,t'}\psi'|| \leqslant ||u_{\omega,t'}|| \cdot ||u_{\omega,t-t'}\psi - \psi'||. \tag{2.8}$$

Put $s = t - t'$. For simplicity, assume that we can write $\psi = \pi(a)\Omega_\omega$ and $\psi' = \pi(a')\Omega_\omega$. In fact, since Ω_ω is cyclic for $\pi_\omega(A)$, we can write ψ as a limit of $\pi(a_\iota)\Omega_\omega$ where (a_ι) is a net in A. A similar result holds for ψ'. In this case we will need an $\epsilon/3$-argument to prove the lemma instead of an $\epsilon/2$-argument which we use now.

Since by (2.3) and (2.4), $u_{\omega,s}\pi(a)\Omega_\omega = \pi(\alpha_s(a))u_{\omega,s}\Omega_\omega = \pi(\alpha_s(a))\Omega_\omega$, it now follows that

$$\begin{aligned} ||u_{\omega,s}\psi - \psi'|| &= ||\pi(\alpha_s(a))\Omega_\omega - \pi(a')\Omega_\omega|| \\ &\leqslant ||\pi(\alpha_s(a))\Omega_\omega - \pi(a)\Omega_\omega|| + ||\pi(a)\Omega_\omega - \pi(a')\Omega_\omega|| \\ &\leqslant ||(\alpha_s(a) - a)|| \cdot ||\Omega_\omega|| + ||\psi - \psi'|| \end{aligned} \tag{2.9}$$

If $\psi \to \psi'$ and $t \to t'$, then we see that the above expression (2.9) converges to zero. Since $u_{\omega,t'}$ is bounded in norm, we conclude that the difference (2.8) goes to zero and therefore we have showed that $(t, \psi) \mapsto u_{\omega,t}\psi$ is continuous. □

Now we are in the position to apply Stone's Theorem to obtain a Hamiltonian h_ω such that

$$u_{\omega,t} = e^{-ith_\omega}, \tag{2.10}$$

where this Hamiltonian h_ω is defined as

$$h_\omega\psi = i\lim_{s\to 0}\frac{u_{\omega,s}-1}{s}\psi = i\frac{d}{ds}\bigg|_{s=0} e^{-ish_\omega}\psi. \tag{2.11}$$

Then,

$$u_{\omega,t}\Omega_\omega = \Omega_\omega, \tag{2.12}$$

immediately implies that

$$h_\omega\Omega_\omega = 0. \tag{2.13}$$

We also have

$$\pi_\omega(\alpha_t(a)) = e^{-ith_\omega}\pi_\omega(a)e^{ith_\omega}. \tag{2.14}$$

2.2 Two different notions of a ground state

We make a link between the notion of a ground state (Definition 2.1) on the local algebra $A_N = B(\mathcal{H}_N)$, with $\mathcal{H}_N$ a finite-dimensional Hilbert space of dimension N, and the notion of a ground state on this algebra in the linear algebra setting, i.e, as an eigenvector or multiple eigenvectors corresponding to the lowest eigenvalue.[2] Take a (self-adjoint) Hamiltonian h acting on $B(\mathcal{H}_N)$. As $\mathcal{H}_N$ is isomorphic as a vector space to the finite-dimensional space $\mathbb{C}^N$, it follows that there exists an ordered orthonormal basis $\{v_0, v_1, ..., v_N\}$ for $\mathcal{H}_N$ consisting of eigenvalues of h.

Consider then the lowest eigenvector v_0 corresponding to the Hamiltonian $h \in B(\mathcal{H}_N)$. We turn v_0 into a state on $B(\mathcal{H}_N)$ by setting

$$\omega_0(a) = \langle v_0, av_0\rangle \ \ (a \in B(\mathcal{H}_N)). \tag{2.15}$$

We claim that this state is a ground state in the sense of Definition 2.1. We denote the the identity operator of $B(\mathcal{H}_N)$ by $\mathbb{1} \equiv \mathrm{id}_{B(\mathcal{H}_N)}$. This is clearly a representation of $B(\mathcal{H}_N)$ on $B(\mathcal{H}_N)$. It follows that we have a triple $(\mathbb{1} : B(\mathcal{H}_N) \to B(\mathcal{H}_N), \mathcal{H}_N, v_0)$, such that

$$\omega_0(a) = \langle v_0, \mathbb{1}(a)v_0\rangle = \langle v_0, av_0\rangle \ \ (a \in B(\mathcal{H}_N)). \tag{2.16}$$

Moreover, v_0 is cyclic for $\mathbb{1}$, as this operator acts as the identity on $B(\mathcal{H}_N)$ and the Hilbert space is finite dimensional.

We are going to apply the GNS-construction to A_N and the state ω_0. In view of Theorem A.9, we find a triple $(\pi_{\omega_0}, \mathcal{H}_{\omega_0}, \Omega_{\omega_0} \equiv [I])$ where $\mathcal{H}_{\omega_0}$ is a Hilbert space, π_{ω_0} a representation of A_N on $\mathcal{H}_{\omega_0}$, such that Ω_{ω_0} is cyclic for π_{ω_0}, and we have

$$\omega_0(a) = \langle [I], [a]\rangle = \langle \Omega_{\omega_0}, \pi_{\omega_0}(a)\Omega_{\omega_0}\rangle. \tag{2.17}$$

By uniqueness of GNS-triples (see again Theorem A.9), we know that a unitary map between both Hilbert spaces $\mathcal{H}_{\omega_0}$ and $\mathcal{H}_N$ exists. In particular, both spaces are isomorphic as vector spaces. We

[2] This construction is general for any state on a C^* algebra and makes use of the GNS-representation. In this paragraph, we give a detailed proof for finite dimensions.

are now going to construct this unitary map that connects both GNS-triples.

Thus we need a bijective map:

$$U : \mathcal{H}_{\omega_0} \to \mathcal{H}_N \tag{2.18}$$

such that

$$\langle U\varphi, U\psi\rangle_{\mathcal{H}_N} = \langle \varphi, \psi\rangle_{\mathcal{H}_{\omega_0}} \quad (\varphi, \psi \in \mathcal{H}_{\omega_0}).$$

Moreover, we want

$$U[I] = U\Omega_{\omega_0} = v_0. \tag{2.19}$$

Notice that for $a \in N_{\omega_0} = \{a \in A_N \mid \omega_0(a^*a) = 0\}$, we have

$$0 = \omega_0(a^*a) = \langle v_0, a^*av_0\rangle = ||av_0||^2. \tag{2.20}$$

Hence

$$[a] = [0] \iff av_0 = 0. \tag{2.21}$$

Write $a \in A_N$ as $a = a|v_0\rangle\langle v_0| + a(\mathbb{1} - |v_0\rangle\langle v_0|)$. Then $[a] = [a|v_0\rangle\langle v_0|]$, since

$$a(\mathbb{1} - |v_0\rangle\langle v_0|)v_0 = a(v_0 - v_0) = 0, \tag{2.22}$$

so that the corresponding equivalence class is the zero class by the above. Hence, an 'operator' in $\mathcal{H}_{\omega_0}$ is determined by its value at v_0.

Now we are going to define U. Take an orthonormal basis $\{[a_i]\}$ for $\mathcal{H}_{\omega_0}$. Since this space is finite-dimensional, it equals the space quotient space H_{ω_0}, explained in Appendix A. Then we define

$$U : \mathcal{H}_{\omega_0} \to \mathcal{H}_N \tag{2.23}$$
$$[a_i] \mapsto a_i v_0. \tag{2.24}$$

This map is well-defined by (2.21). We will see that U is unitary. Note that the adjoint U^* is given by

$$U^* : H_{\Lambda_N} \to \mathcal{H}_{\omega_0} \tag{2.25}$$
$$v_i \mapsto [a_i], \tag{2.26}$$

which is well-defined as well since it defined on basis vectors of $\mathcal{H}_N$. It follows that $a_iv_0 = v_i$. How is this possible?
Note that $A_N = B(\mathcal{H}_N)$ is a unital C^*- algebra and ω_0 is a state on A_N. As $\Omega_0 = [I]$ is cyclic for π_{ω_0}, we have

$$\pi_{\omega_0}(A_N)\Omega_{\omega_0} = \mathcal{H}_{\omega_0}, \tag{2.27}$$

so that

$$U(\pi_{\omega_0}(A_N)\Omega_{\omega_0}) = U(\mathcal{H}_{\omega_0}) = H_{\Lambda_N}. \tag{2.28}$$

Then for each $v_i \in \mathcal{H}$, we have

$$v_i = U(\pi_{\omega_0}(a_i)\Omega_{\omega_0}) = U[a_i\Omega_{\omega_0}] = a_iv_0. \tag{2.29}$$

Note that for arbitrary C^*-algebras A, one needs to take the closure of the space $\pi_{\omega_0}(A_N)\Omega_{\omega_0}$. The result remains true when A does not have a unit. In that case, it has an approximate unit.

It is an easy exercise to see that U is an isometry:

$$\langle U([a_i]), U([a_j])\rangle = \langle a_i v_0, a_j v_0\rangle = \omega_0(a_i^* a_j) = \langle [a_i], [a_j]\rangle. \tag{2.30}$$

It follows that U is injective. Since we already know that such a unitary map exists, both (finite) dimensions of $\mathcal{H}_N$ and $\mathcal{H}_{\omega_0}$ are equal. Therefore, injectivity implies surjectivity. This shows that U is unitary.

Note that by construction:

$$U^*(av) = \pi_{\omega_0}(a)(U^* v). \tag{2.31}$$

In particular, for the bounded operator[3] h, we find

$$U^*(e^{ith} v) = \pi_{\omega_0}(e^{ith}) U^*(v). \tag{2.32}$$

We also have that $U[I] = v_0$. Since $a_0 v_0 = v_0$, we have by the above $(a_0 - \mathbb{1})v_0 = 0$, so that $[a_0 - I] = [0]$, hence $[a_0] = [I]$. Therefore, indeed,

$$U[I] = U[a_0] = v_0. \tag{2.33}$$

Now, we are going to define a time evolution on all relevant spaces using again Theorem A.9 and Theorem A.10. We define, for given $h^* = h \in B(\mathcal{H}_N)$,

$$\text{on } \mathcal{H}_N;\ u_t : v \mapsto e^{ith} v \tag{2.34}$$

$$\text{on } A_N = B(\mathcal{H}_N);\ \alpha_t : a \mapsto e^{-ith} a e^{ith} \tag{2.35}$$

$$\text{on } \mathcal{H}_{\omega_0};\ [a] \mapsto u_s([a]), \tag{2.36}$$

such that $u_s[I] = [I]$, and $\pi_{\omega_0}(\alpha_s(a)) = u_s \pi_{\omega_0}(a) u_s^*$. Recall that this u_s is defined through

$$u_s[a] = u_s \pi_{\omega_0}(a)[I] = \pi_{\omega_0}(\alpha_s(a))[I] = [\alpha_s(a)]. \tag{2.37}$$

Note that the above is possible since for each $t \in \mathbb{R}$, the triple $(\pi_{\omega_0} \circ \alpha_t, \mathcal{H}_{\omega_0}, \Omega_{\omega_0})$ is another GNS triple (as follows from an easy computation).

By Lemma 2.2, the family of unitaries u_s om $\mathcal{H}_{\omega_0}$ forms a continuous representation of $\mathbb{R}$. In particular, it is a strongly continuous one-parameter subgroup. We may therefore apply Stone's theorem to find a Hamiltonian h_{ω_0} on $\mathcal{H}_{\omega_0}$ such that

$$h_{\omega_0}[a_i] = i \lim_{s\to 0} \frac{u_s - I}{s}[a_i] = i \lim_{s\to 0} \frac{[\alpha_s(a_i)] - [a_i]}{s}. \tag{2.38}$$

But $[\alpha_t(a_i)] = [e^{-ith} a_i e^{ith}]$, and $e^{-ith} a_i e^{ith} v_0 = e^{-ith} a_i e^{it\lambda_0} v_0 = e^{it\lambda_0} e^{-ith} a_i v_0$, so that

$$\begin{aligned}
[\alpha_t(a_i)] &= e^{it\lambda_0} U^*(e^{-ith} v_i) \\
&= U^*(e^{-it(h-\lambda_0)} v_i) \\
&= U^*(e^{-it(\lambda_i - \lambda_0)} v_i) \\
&= e^{-it(\lambda_i - \lambda_0)} U^*(v_i) \\
&= e^{it\lambda_i - \lambda_0}[a_i].
\end{aligned} \tag{2.39}$$

[3] In infinite dimensions, this result is not true. Consider for example an unbounded Hamiltonian and the algebra of compact operators.

Then we obtain

$$\begin{aligned} h_{\omega_0}[a_i] &= i \lim_{s\to 0} \frac{[\alpha_s(a_i)] - [a_i]}{s} \\ &= i \lim_{s\to 0} \frac{[e^{-is(\lambda_i-\lambda_0)}a_i] - [a_i]}{s} \\ &= (\lambda_i - \lambda_0)[a_i]. \end{aligned} \tag{2.40}$$

It is clear that h_ω is positive precisely if λ_0 is the smallest eigenvalue.

One can show that the map $\alpha : \mathbb{R} \to \mathrm{Aut}(A_{\Lambda_N}),\ t \mapsto \alpha_t$ defines a strongly continuous one-parameter subgroup of automorphisms, i.e., a time evolution. Thus (A_{Λ_N}, α) is a C^*-dynamical system (see text preceding Definition 2.1).

We still have to check that ω_0 is invariant under α_t. This is easy:

$$\begin{aligned} \omega_0(\alpha_t(a)) &= \langle v_0, u_t a(u_t)^* v_0 \rangle \\ &= \langle e^{-ith} v_0, a e^{-ith} v_0 \rangle \\ &= e^{-it\lambda_0} e^{+it\lambda_0} \langle v_0, a v_0 \rangle \\ &= \omega_0(a). \end{aligned} \tag{2.41}$$

Thus we have shown that, given a self-adjoint Hamiltonian h on $\mathcal{H}_N$, we can construct a C^*-dynamical system $A_N = B(\mathcal{H}_N)$, a time evolution $\alpha : \mathbb{R} \to \mathrm{Aut}(A_N)$ and a time-independent state ω_0. Moreover, we can construct a continuous unitary representation u_s on $\mathcal{H}_\omega$ such that (by Stone) there exists a Hamiltonian with positive spectrum. Hence ω_0 is a ground state for the dynamical system in the sense of Definition 2.1.

Conversely, suppose we are given a state ω on $B(\mathcal{H}_N)$, with $\mathcal{H}_N$ a finite-dimensional Hilbert space, and a one-parameter subgroup $\alpha : \mathbb{R} \to \mathrm{Aut}(A_N),\ t \mapsto \alpha_t$. This gives rise to a Hamiltonian h_ω and a cyclic unit vector Ω_ω such that $h_\omega \Omega_\omega = 0$, as we have just seen. Then, using the same definition of U, we have $U\Omega_\omega = v_0$. We can recover a Hamiltonian h on $B(H_{\Lambda_N})$ by putting $h\psi = hU(\varphi) = U(h_\omega(\varphi))$, where $\psi \in D(h)$ such that $\psi = U(\varphi)$ $(\varphi \in D(h_\omega))$. Here, $D(h)$ is defined as $D(h) = U(D(h_\omega))$, being the domain of h.
Then,

$$hv_0 = hU(\Omega_\omega) = U(h_\omega(\Omega_\omega)) = U(0) = 0. \tag{2.42}$$

The next step is to define a notion of spontaneous symmetry breaking for C^*-dynamical systems.

2.3 Spontaneous symmetry breaking

In this thesis we use the standard notion of symmetry breaking in algebraic quantum theory taken from [22, p.379]. Given a C^*-algebra A, we denote the state space of A, by $S(A)$, and its extreme boundary by $\partial_e S(A)$. The set of ground states of some given time-evolution α, then forms a compact convex subset of $S(A)$, denoted by $S_0(A)$. The subscript 0 in $S_0(A)$, historically corresponds to temperature $T = 0$, or equivalently $\beta = \infty$ for $\beta = 1/T$. Moreover, we assume that

$$\partial_e S_0(A) = S_0(A) \cap \partial_e S(A). \tag{2.43}$$

This means that pure ground states (i.e., $\omega \in \partial_e S_0(A)$) are pure states as well as ground states (i.e., $\omega \in \partial_e S(A)$ and $\omega \in S_0(A)$) . This is indeed the case for $A = B(H)$, with H a separable Hilbert space.

Definition 2.3. *Spontaneous symmetry breaking. (SSB)*
Suppose we have a C^*-algebra A, a time evolution α, a group G, and a homomorphism $\gamma : G \to Aut(A)$, which is a symmetry of the dynamics α in that

$$\alpha_t \circ \gamma_g = \gamma_g \circ \alpha_t \quad (g \in G, t \in \mathbb{R}). \tag{2.44}$$

The G-symmetry is said to be spontaneously broken (at temperature $T = 0$) if

$$(\partial_e S_0(A))^G = \varnothing, \tag{2.45}$$

and weakly broken if $(\partial_e S_0(A))^G \neq \partial_e S_0(A)$, i.e., there is at least one $\omega \in \partial_e S_0(A)$ that fails to be G-invariant (although invariant extreme ground states may exist).

Here $\mathscr{S}^G = \{\omega \in \mathscr{S} |\ \omega \circ \gamma_g = \omega\ \forall g \in G\}$, defined for any subset $\mathscr{S} \in S(A)$, is the set of G- invariant states in $\mathscr{S}$. Assuming (2.43), then (2.45) means that there are no G-invariant pure ground states. This means also that if spontaneous symmetry breaking occurs, then invariant ground states are not pure. In the next paragraph, we will give an important example.

2.4 Quantum mechanical symmetric double well model versus its classical limit

In this section we first consider the quantum Hamiltonian that describes a particle in a symmetric double well. We take $G = \mathbb{Z}_2$ as our symmetry group. The goal is to show that its ground state does not break the $\mathbb{Z}_2$-symmetry in the sense of Definition 2.3. However, we will see that the ground state in the classical limit system does break the $\mathbb{Z}_2$-symmetry.

Let us focus first on the quantum mechanical system. We take $B_0(L^2(\mathbb{R}))$ as C^*-algebra of observables on the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$.[4] Take $m = 1/2$ and put the symmetric double well potential $V(x) = \frac{1}{4}\lambda(x^2 - a^2)^2$ in the Hamiltonian

$$h_\hbar = -\hbar^2 \frac{d^2}{dx^2} + V(x). \tag{2.46}$$

Here $a = \beta/\sqrt{\lambda} > 0$, whilst $\pm a$ denotes the position of the both minima in the potential, and β is a positive constant. The Hamiltonian is an unbounded operator, and is a map

$$h_\hbar : D(h_\hbar) \to L^2(\mathbb{R}), \tag{2.47}$$

where $D(h_\hbar)$ is a dense domain of $L^2(\mathbb{R})$.

As we have said, we want to show that spontaneous symmetry breaking (SSB) is typically not happening in quantum mechanics, because the ground state is usually unique in finite quantum systems[5], like for this one-particle system describing a particle in a symmetric double well. In order to show that this quantum system does not display SSB, we show that for the group $G = \mathbb{Z}_2$, a homomorphism $\gamma : G \to \mathrm{Aut}(B_0(L^2(\mathbb{R})))$ and a time evolution $\alpha : \mathbb{R} \to \mathrm{Aut}(B_0(L^2(\mathbb{R})))$, such that γ is a symmetry of the dynamics, this G-symmetry is not spontaneously broken, in that

$$(\partial_e S_0(A))^G \neq \varnothing. \tag{2.48}$$

[4]The algebra $B_0(L^2(\mathbb{R}))$ denotes the C^*-algebra of compact operators.

[5]This is not always true: the ground state of the finite quantum Ising model without magnetic field interaction is doubly degenerate.

As said before, we take $B_0(L^2(\mathbb{R}))$ as our C^*-algebra, and the group $G = \mathbb{Z}_2$ is identified with the set $\{1, -1\}$. We then define the homomorphism by

$$\begin{aligned}
&\gamma : \{1,-1\} \to \mathrm{Aut}(B_0(L^2(\mathbb{R}))),\\
&1 \mapsto \gamma_1,\\
&\gamma_1(a) = a \qquad (2.49)\\
& \qquad (2.50)\\
&-1 \mapsto \gamma_{-1},\\
&\gamma_{-1}(a) = \tau a \tau^*, \quad (a \in B_0(L^2(\mathbb{R})))\\
&\tau : L^2(\mathbb{R}) \to L^2(\mathbb{R}),\\
&f \mapsto \tau(f), \quad (f \in L^2(\mathbb{R}))\\
&\tau(f)(x) = f(-x) \quad (x \in \mathbb{R}). \qquad (2.51)
\end{aligned}$$

We define a time evolution by

$$\begin{aligned}
&\alpha : \mathbb{R} \to \mathrm{Aut}(B_0(L^2(\mathbb{R}))),\\
&t \mapsto \alpha_t,\\
&\alpha_t(a) = e^{ih_\hbar t} a e^{-ih_\hbar t}. \qquad (2.52)
\end{aligned}$$

It follows that $(B_0(L^2(\mathbb{R})), \alpha)$ is a C^*-dynamical system. Now we show that the homomorphism is a symmetry of the dynamics, i.e. that

$$\alpha_t \circ \gamma_g = \gamma_g \circ \alpha_t. \qquad (2.53)$$

So we have to show:

$$\gamma_g \circ \alpha_t(f)(x) = \alpha_t \circ \gamma_g(f)(x), \quad \forall f \in L^2(\mathbb{R}) \quad x \in \mathbb{R} \qquad (2.54)$$

This is clear for $g = 1$, as γ_1 acts as the identity map, so that γ_1 commutes with $h_\hbar$ and hence also with all powers of $h_\hbar$, and thus with $e^{ih_\hbar t}$.
It is also clear for $g = -1$, as τ obviously commutes with the second derivative operator (it takes twice a minus sign) and also with the potential because of the quadratic term. So τ commutes with the Hamiltonian and hence with the exponential $e^{ih_\hbar t}$.
So indeed, we have a $\mathbb{Z}_2$-symmetry. It turns out that this $\mathbb{Z}_2$-symmetry is not spontaneously broken, as we will show later in this paragraph. First, we need to define a ground state in the sense of Definition 2.1.

The ground state eigenfunction $\psi_\hbar^0$ corresponding to this system is unique, as follows from an infinite-dimensional version of the Perron-Frobenius Theorem. Furthermore, one can show that the bottom of the spectrum of the quantum Hamiltonian $h_\hbar$ is an eigenvalue. We will give a detailed proof of both facts in Chapter 5. In view of Definition 2.1, we convert $\psi_\hbar^0$ into a state on the C^* algebra $A = B_0(L^2(\mathbb{R}))$. An obvious choice is to turn it into a vector state:

$$\omega_0(a) = \langle \psi_\hbar^0, a\psi_\hbar^0 \rangle \quad (a \in B_0(L^2(\mathbb{R}))). \qquad (2.55)$$

We claim that this state is a ground state in the sense of Definition 2.1, and show that this is in fact *the* ground state of the C^*-dynamical system (A, α). Note first that the invariance of ω_0 under α_t is obvious. We denote the identity operator of $B_0(L^2(\mathbb{R}))$ by $\mathbb{1} \equiv \mathrm{id}_{B_0(L^2(\mathbb{R}))}$. This is clearly a representation of A on $\mathcal{H} = L^2(\mathbb{R})$. It follows that we have a triple $(\mathbb{1} \equiv \mathrm{id}_{B_0(L^2(\mathbb{R}))} : A \to A, L^2(\mathbb{R}), \psi_\hbar^0)$, such that

$$\omega_0(a) = \langle \psi_\hbar^0, \mathbb{1}(a)\psi_\hbar^0 \rangle = \langle \psi_\hbar^0, a\psi_\hbar^0 \rangle \quad (a \in B_0(L^2(\mathbb{R}))). \qquad (2.56)$$

We normalize $\psi_\hbar^{(0)}$. It follows that $\psi_\hbar^{(0)}$ is cyclic for $\mathbb{1}$. To see this, note first that $\mathbb{1}$ acts as the identity on $A = B_0(L^2(\mathbb{R}))$. Then, given a $\varphi \in L^2(\mathbb{R})$, put $a = |\varphi\rangle\langle\psi_\hbar^{(0)}| \in A$. It follows that

$$a\psi_\hbar^{(0)} = \varphi. \tag{2.57}$$

Therefore, indeed $\psi_\hbar^{(0)}$ is cyclic for $\mathbb{1}$.

Similarly as for the finite-dimensional case, explained in §2.2, we apply the GNS-construction (see e.g. Theorem A.9) to $A = B_0(L^2(\mathbb{R}))$ and the state ω_0. From this construction, we find another triple $(\pi_{\omega_0}, \mathcal{H}_{\omega_0}, \Omega_{\omega_0} = \lim_\lambda [e_\lambda])$, where $\mathcal{H}_{\omega_0}$ is a Hilbert space, $\pi_{\omega_0} : A \to B(\mathcal{H}_{\omega_0})$ is the GNS-representation of A on $\mathcal{H}_{\omega_0}$, and $\Omega_{\omega_0} \in \mathcal{H}_{\omega_0}$ is a cyclic unit vector for π_{ω_0}.[6] We also have

$$\omega_0(a) = \langle [I], [a] \rangle = \langle \Omega_{\omega_0}, \pi_{\omega_0}(a)\Omega_{\omega_0} \rangle. \tag{2.58}$$

By Theorem A.9, we know that a unitary map $U : L^2(\mathbb{R}) \to \mathcal{H}_{\omega_0}$ exists, and thus $L^2(\mathbb{R})$ is isomorphic to $\mathcal{H}_{\omega_0}$. The next step is to define this U. The procedure is analogous to the finite-dimensional case, except that one detail is different.[7] As $L^2(\mathbb{R})$ is separable, we can take an orthonormal basis $\{\psi_i\}_{i\in\mathbb{N}}$, starting with $\psi_0 = \psi_\hbar^0$. Since $L^2(\mathbb{R})$ and $\mathcal{H}_{\omega_0}$ are isomorphic, the latter space is separable as well. Then, since the vector space $H_{\omega_0} \equiv \pi_{\omega_0}(A)\Omega_{\omega_0}$ is a dense subspace of $\mathcal{H}_{\omega_0}$, we first define U on this subspace,

$$U : H_{\omega_0} \to L^2(\mathbb{R}) \tag{2.59}$$

$$[a_i] \mapsto a_i\psi_0. \tag{2.60}$$

This map is well-defined because, if $[a_i] = [a_j]$, then by definition of ω_0, it follows that $(a_i - a_j)\psi_0 = 0$, so that

$$U[a_i] = U[a_j]. \tag{2.61}$$

Then U is an isometry which follows from the computation:

$$\langle [a_i], [a_j] \rangle = \omega_0(a_i^* a_j) = \langle a_i\psi_0, a_j\psi_0 \rangle = \langle U[a_i], U[a_j] \rangle. \tag{2.62}$$

Therefore, U extends linearly to $\mathcal{H}_{\omega_0}$ by continuity. Its image is then the closure of $\mathbb{1}(a)\psi_0$, which is $L^2(\mathbb{R})$, since ψ_0 is cyclic for $\mathbb{1}$. Thus U is surjective and hence, in view of (2.62), unitary.

We will now show that the basis vectors ψ_i are related to ψ_0, via

$$\psi_i = \lim_\lambda a_i^{(\lambda)}\psi_0 \quad (i \in \mathbb{N}), \tag{2.63}$$

where $\{a_i^{(\lambda)}\}_\lambda$ is a net in A. To show this, we use the fact that

$$\overline{\pi_{\omega_0}(A)\Omega_{\omega_0}} = \mathcal{H}_{\omega_0}, \tag{2.64}$$

so that

$$U(\overline{\pi_{\omega_0}(A)\Omega_{\omega_0}}) = L^2(\mathbb{R}). \tag{2.65}$$

[6] Since positive linear functionals are bounded, it follows that the equivalence class of the net $\{e_\lambda\}_\lambda$ converges to a cyclic unit vector Ω_{ω_0} in H_{ω_0}, where $\{e_\lambda\}_\lambda$ is an approximate identity for the non-unital algebra A.

[7] This general GNS-construction is true for any state defined on a C^*-algebra. We give a detailed derivation for this specific algebra and use some of its properties. For example, the fact that $\psi_\hbar^{(0)}$ is cyclic for $\mathbb{1}$ and ω_0 is pure, is a result of the properties of $B_0(L^2(\mathbb{R}))$.

Note that $A = B_0(L^2(\mathbb{R}))$ is not finite dimensional, so that we really need to take the closure of H_{ω_0} in order to obtain $\mathcal{H}_{\omega_0}$. We compute for each $\psi_i \in L^2(\mathbb{R})$:

$$\psi_i = U(\lim_\lambda \pi_{\omega_0}(a_i^{(\lambda)})\Omega_{\omega_0}) = \lim_\lambda U(\pi_{\omega_0}(a_i^{(\lambda)})\Omega_{\omega_0}) = \lim_\lambda U[a_i^{(\lambda)}] = \lim_\lambda a_i^{(\lambda)}\psi_0. \tag{2.66}$$

This shows that (2.63) holds. In particular, by taking an approximate identity $\{e_\lambda\}_\lambda$ for $A = B_0(L^2(\mathbb{R}))$, it follows that

$$U\Omega_{\omega_0} = U\lim_\lambda \pi_{\omega_0}(e_\lambda)\Omega_{\omega_0} = \lim_\lambda e_\lambda\psi_0 = \psi_0. \tag{2.67}$$

For the time evolution on all relevant spaces, we define, for given $h_\hbar = h_\hbar^*$

$$\text{on } L^2(\mathbb{R});\ u_t : \psi \mapsto e^{ith_\hbar}\psi \tag{2.68}$$

$$\text{on } A = B_0(L^2(\mathbb{R}));\ \alpha_t : a \mapsto e^{-ith_\hbar}ae^{ith_\hbar} \tag{2.69}$$

$$\text{on } \mathcal{H}_{\omega_0};\ [a] \mapsto u_s([a]). \tag{2.70}$$

Again, in view of Theorem A.10, the unitary operator u_s is defined by

$$u_s\pi_{\omega_0}(a)\Omega_{\omega_0} = \pi_{\omega_0}(\alpha_s(a))\Omega_{\omega_0}. \tag{2.71}$$

By Lemma 2.2, the family of unitaries u_s on $\mathcal{H}_{\omega_0}$ forms a continuous representation of $\mathbb{R}$. In particular, it is a strongly continuous one parameter subgroup. We may therefore apply Stone's Theorem to find a Hamiltonian h_{ω_0} on $\mathcal{H}_{\omega_0}$ such that

$$h_{\omega_0}\varphi = i\lim_{s\to 0}\frac{u_s - I}{s}\varphi = i\lim_{s\to 0}\frac{\lim_\lambda (u_s - I)[a^{(\lambda)}]}{s}. \tag{2.72}$$

where $\varphi \in \mathcal{H}_{\omega_0}$ is of course given by the norm-limit:

$$\varphi = \lim_\lambda [a^{(\lambda)}]. \tag{2.73}$$

Take a basis vector $\varphi_i \in \mathcal{H}_{\omega_0}$, and compute

$$\begin{aligned}
u_s\varphi_i &= \lim_\lambda u_s([a_i^{(\lambda)}]) \\
&= \lim_\lambda [\alpha_s(a_i^{(\lambda)})] \\
&= \lim_\lambda \pi_{\omega_0}(e^{-ish_\hbar}a_i^{(\lambda)}e^{ish_\hbar})U^*\psi_0 \\
&= \lim_\lambda U^*(e^{-ish_\hbar}a_i^{(\lambda)}e^{ish_\hbar}\psi_0) \\
&= \lim_\lambda U^*e^{is\lambda_0}(e^{-ish_\hbar}a_i^{(\lambda)}\psi_0) \\
&= U^*e^{is\lambda_0}(e^{-ish_\hbar}\lim_\lambda a_i^{(\lambda)}\psi_0) \\
&= U^*(e^{-is(\lambda_i-\lambda_0)}\psi_i) \\
&= e^{-is(\lambda_i-\lambda_0)}\varphi_i.
\end{aligned} \tag{2.74}$$

We used that $e^{-ish_\hbar}a_i^{(\lambda)}e^{ish_\hbar} \in B_0(L^2(\mathbb{R}))$, since this algebra is an ideal. In the final last step we applied (2.63). We obtain

$$h_{\omega_0}\varphi_i = i\lim_{s\to 0}\frac{e^{-is(\lambda_i-\lambda_0)}\varphi_i - \varphi_i}{s} = (\lambda_i - \lambda_0)\varphi_i. \tag{2.75}$$

It is clear that h_ω is positive precisely if λ_0 is the smallest element, being an eigenvalue as well, of the spectrum of $h_\hbar$. But as we have already mentioned, it is true by a deep result based on compactness of the resolvent operator (explained in Chapter 5) that indeed $h_\hbar$ admits an eigenvalue at the bottom of its spectrum. Hence $\sigma(h_\omega) \subset \mathbb{R}^+$.

We have shown that given a self-adjoint Hamiltonian $h_\hbar$ on $L^2(\mathbb{R}^2)$, we can make a C^*-dynamical system $A = B_0(H)$, a time evolution $\alpha : \mathbb{R} \to \mathrm{Aut}(A)$ and a state ω such that this state is time-independent. Moreover we can make a continuous unitary representation u_s on $\mathcal{H}_{\omega_0}$ such that there exists (by Stone) a Hamiltonian which has positive spectrum. Hence ω_0 is a ground state for the given C^* -dynamical system.

So far, we have transformed the ground state eigenfunction $\psi_\hbar^0$ of norm one into a ground state in the sense of Definition 2.1, implicitly using the fact that $\psi_\hbar^0$ is a vector state on the algebra of compact operators, and hence is a pure state. Since we have already shown that we have a $\mathbb{Z}_2$-symmetry, we are now in a position to use Definition 2.3. We will show that the $\mathbb{Z}_2$-symmetry is not spontaneously broken.

This is now an easy corollary: uniqueness of the ground state eigenfunction $\psi_\hbar^0$ implies, of course, that its corresponding vector state ω_0 is unique as well. Therefore, we have

$$\partial_e S_0(B_0(L^2(\mathbb{R}))) = \{\omega_0\}. \tag{2.76}$$

It follows that $\omega_0 \circ \gamma_g = \omega_0$, for all $g \in \mathbb{Z}_2$. We show this by contradiction: if there would exists an element $g \in \mathbb{Z}_2$ such that $\omega_0 \circ \gamma_g \neq \omega_0$, then we can find a compact operator $\tilde{a}$ for which this inequality holds. Note that g has to be -1, as $g = 1$ acts as the identity. Then

$$\omega_0(\gamma_{-1}(\tilde{a})) = \langle \psi_\hbar^0, \gamma_{-1}(\tilde{a})\psi_\hbar^0 \rangle = \langle \tau^*\psi_\hbar^0, \tilde{a}\tau^*\psi_\hbar^0 \rangle = |z|^2 \langle \psi_\hbar^0, \tilde{a}\psi_\hbar^0 \rangle = \omega_0(\tilde{a}), \tag{2.77}$$

where we used the fact that $\psi_\hbar^0$ is an eigenfunction of τ as well since τ commutes with $h_\hbar$, and the ground state is unique. The number z is a scalar with absolute value equal to one. Therefore, we have a contradiction. Hence we conclude

$$\partial_e S_0(B_0(L^2(\mathbb{R})))^G = \{\omega_0\} \neq \varnothing. \tag{2.78}$$

Thus the G-symmetry is not spontaneously broken, because the ground state is unique.

Now we turn to the SSB classical mechanics. The ensuing Hamiltonian is given by

$$h_0(p, q) = p^2 + V(q), \tag{2.79}$$

where V the double well potential as defined above. We take $A = C_0(\mathbb{R}^2)$ as the C^*-algebra of observables on the phase space $\mathbb{R}^2$. As a homomorphism acting on the group $G = \mathbb{Z}_2$, we take

$$\begin{aligned} &\gamma : \mathbb{Z}_2 \to \mathrm{Aut}(C_0(\mathbb{R}^2)), \\ &\pm 1 \mapsto \gamma_{\pm 1}, \\ &\gamma_{\pm 1}(f)(p, q) = f(\pm p, \pm q), \ (f \in C_0(\mathbb{R}^2, (p, q) \in \mathbb{R}^2. \end{aligned} \tag{2.80}$$

We define a time evolution by

$$\begin{aligned} &\alpha : \mathbb{R} \to \mathrm{Aut}(C_0(\mathbb{R}^2)), \\ &t \mapsto \alpha_t, \\ &\alpha_t(f)(p, q) = f(\varphi_t^{h_0}(p, q)), \ (f \in C_0(\mathbb{R}^2), (p, q) \in \mathbb{R}^2). \end{aligned} \tag{2.81}$$

Here $\varphi_t^{h_0}$ denotes the (unique) maximal flow of the Hamiltonian vector field X^{h_0}, uniquely induced by the classical Hamiltonian h_0.[8] The point $\varphi_t^{h_0}(p,q)$ denotes the starting point of the time evolution. In order to apply Definition 2.3, we first have to check that

$$\gamma_g \circ \alpha_t(f) = \alpha_t \circ \gamma_g(f) \tag{2.82}$$

Evaluating this at $(p,q) \in \mathbb{R}^2$ and using the definition of α_t, we must show that

$$f(\varphi_t^{h_0}(p,q)) = \gamma_1(f)(\varphi_t^{h_0}(p,q)), \quad \text{and} \tag{2.83}$$

$$f(\varphi_t^{h_0}(-p,-q)) = \gamma_{-1}(f)(\varphi_t^{h_0}(p,q)). \tag{2.84}$$

It is clear that (2.83) is true by definition of γ_1. For (2.84), if we denote $(p',q') = \varphi_t^{h_0}(p,q)$, then we need to show that

$$(-p',-q') = \varphi_t^{h_0}(-p,-q), \tag{2.85}$$

since then (2.84) reads

$$f(\varphi_t^{h_0}(-p,-q)) = f(-p',-q') = \gamma_{-1}(f)(p',q'), \tag{2.86}$$

which directly implies that $\gamma_{-1}(f)(\varphi_t^{h_0}(p,q)) = f(\varphi_t^{h_0}(-p,-q))$.

To prove this, we define $\tilde{\gamma} : \mathbb{R}^2 \to \mathbb{R}^2$ by $(p,q) \mapsto (-p,-q)$. So $\gamma_{-1} = \tilde{\gamma}^*$. It follows by definition of the Hamiltonian that

$$h_0 \circ \tilde{\gamma} = h_0. \tag{2.87}$$

We need a lemma in order to prove (2.85).

Lemma 2.4. *If $t \mapsto (p(t),q(t))$ is an integral curve for X^{h_0}, then also $t \mapsto \tilde{\gamma}_{(p(t),q(t))}$ is an integral curve for X^{h_0}.*

Proof. Put $z(t) = (p(t),q(t))$. Then

$$(\tilde{\gamma} \circ z)(t) = \tilde{\gamma}(z(t)) = (-p(t),-q(t)) = -z(t). \tag{2.88}$$

By assumption, we have

$$X^{h_0}_{z(t)} = \frac{d}{dt} z(t). \tag{2.89}$$

It follows that

$$X^{h_0}_{(\tilde{\gamma}\circ z)(t)} = X^{h_0}_{-z(t)} = \frac{d}{dt}\Big(-z(t)\Big) = \frac{d}{dt}(\tilde{\gamma} \circ z)(t), \tag{2.90}$$

where in the first step we used the invariance of h_0 under $\tilde{\gamma}$. □

We conclude that if (p',q') flows to (p,q) according to h_0, then $\tilde{\gamma}(p',q')$ flows to $\tilde{\gamma}(p,q)$ again according to h_0. This is precisely what (2.85) means.

So we know that the time evolution α_t commutes with γ_g for all $g \in G$. Moreover, one can easily show that the map $\alpha : \mathbb{R} \to \mathrm{Aut}(C_0(\mathbb{R}^2))$, $t \mapsto \alpha_t$ defines a time evolution, using the fact

[8] The differentiable function $h_0 : \mathbb{R}^2 \to \mathbb{R}$, defined on the symplectic manifold $\mathbb{R}^2$, determines a unique vector field X^{h_0}, by defining for every vector Y on $\mathbb{R}^2$, $dh_0(Y) = \omega(X^{h_0}, Y)$, where ω is the standard one-form on $\mathbb{R} \times \mathbb{R}$ given by the determinant.

that the flow is a smooth map from $\mathbb{R} \times C_0(\mathbb{R}^2) \to C_0(\mathbb{R}^2)$. It follows that $(C_0(\mathbb{R}^2), \alpha)$ is a C^*-dynamical system.

We still need to find a ground state in the sense of Definition 2.1 such that it breaks the symmetry in the sense of Definition 2.3, as we have claimed in the beginning of this paragraph. For classical systems (i.e. with A a commutative C^*-algebra) this definition means that the integral curve $t \mapsto x_0(t) \in \mathbb{R}^2$ of the Hamiltonian vector field X^{h_0}, satisfies

$$\begin{aligned} &1.\ x_0(t) = x_0 \ \text{ for all } t \in \mathbb{R}; \\ &2.\ h_{\omega_0}(x_0) \geqslant 0, \end{aligned} \tag{2.91}$$

as we will see below.[9] Condition 1 is equivalent to the statement $dh_0 = 0$. Hence, extreme points of h_0 correspond to ground states of this classical system. These are not necessarily the minima of h_0. In particular, Definition 2.1 is not applicable for classical systems since all extreme points are considered as ground states. Nonetheless, we will only take the minima of h_0 as classical ground state since it is well-known (from e.g. [22, sec. 10.1]) that *only* these points, corresponding to the minima of the potential, form the actual ground state. Moreover, we will explain that the Hamiltonian h_{ω_0} obtained from the GNS-construction, equals the zero operator, so that statement 2 above is empty. First, we show that the $\mathbb{Z}_2$-symmetry is broken by Dirac measures $\mu_0^{\pm}$, i.e., that there exists a $g \in G$ such that

$$\mu_0^{\pm}(\gamma_g(f)) \neq \mu_0^{\pm}(f) \tag{2.92}$$

We need the following lemma.

Lemma 2.5. *$\mu_0^{\pm}$ is the doubly degenerate ground state of the classical Hamiltonian h_0.*

Proof. Note that by the above, the ground states are obtained by extremizing the classical Hamiltonian, that is

$$\nabla h_0(p, q) = (2p, \lambda(q^2 - a^2)q). \tag{2.93}$$

This is zero if and only if $p = 0$ and $q \in \{0, \pm a\}$. As we have said, we ignore the point $(0, 0)$, since it is not a minimum. The minima instead are obtained if $h_{pp} > 0$ and $h_{qq} > 0$, which is achieved only for $p = 0$ and $q = \pm a$. Keep still in mind that this does not follow from Definition 2.1. Thus the ground states in the 'classical' sense are given by the points $(0, a)$ and $(0, -a)$. Now we use the fact that for any locally compact space X, the states on $C_0(X)$ bijectively correspond with complete regular probability measures on X, according to

$$\mu(f) = \int_X d\mu(f). \tag{2.94}$$

In particular, points (p, q) in phase space correspond with Dirac measures $\delta_{(p,q)}$. Hence

$$\mu_0^{\pm}(f) := \delta_{(0,\pm a)}(f) = \int_{\mathbb{R}^2} d\mu_{(0,\pm a)}(f) = f(0, \pm a). \tag{2.95}$$

We have to check that this is indeed a ground state à la Definition 2.1.

We are working with the C^* - dynamical system $A = (C_0(\mathbb{R}^2), \alpha)$, where $\alpha_t(f) = (\varphi_t^{h_0})^*(f) = f \circ \varphi_t^{h_0}$. Moreover, it is clear that Dirac measures $\mu_0^{\pm}$ are pure states.

[9] Note that the equivalence between this definition and Definition 2.1 is based on the fact the points in phase space bijectively correspond with Dirac measures.

Consider $\mu_0^{\pm}$. Apply the GNS-construction to A to find a Hilbert space $\mathcal{H}_{\mu_0^{\pm}} = \overline{A/\sim}$, with $f \sim 0 \iff \mu_0^{\pm}(f^*f) = 0$. But, $\mu_0^{\pm}(f^*f) = |f(0,\pm a)|^2$, hence $f \sim 0 \iff f(0,\pm a) = 0$.[10]

We claim that the corresponding Hamiltonian $h_{\mu_0^{\pm}}$, obtained from the GNS-construction, is the zero operator. Therefore, we consider the Hamiltonian vector field X^{h_0} induced by the classical Hamiltonian. It is easy to show that

$$X^{h_0} = \left(\frac{\partial V}{\partial q}, -p\right) = \Big(\lambda q(q^2 - a^2), -p\Big). \tag{2.96}$$

Then, $X^{h_0}(0,\pm a) = (0,0)$, i.e., the vector field vanishes at $(0,\pm a)$. The flow $(p(t), q(t))$ such that $(\dot{p}(t), \dot{q}(t)) = X^{h_0}(p(t), q(t))$ and $p(0) = 0$ and $q(0) = \pm a$, at the point $(0,\pm a)$ is simply given by $(0,\pm a)$, so that

$$\mu_0^{\pm}(\alpha_t(f)) = \alpha_t(f)(0,\pm a) = f(\varphi_{-t}^{h_0}(0,\pm a)) = f(0,\pm a) = \mu_0^{\pm}(f). \tag{2.97}$$

Thus, both states $\mu_0^{\pm}$ are time independent. Moreover, in view of Definition 2.1 again, the unitary map u_s is

$$u_s[f] = [\alpha_s(f)] = [f], \tag{2.98}$$

as $(0,\pm a)$ is stationary for X^{h_0} and use the equivalence relation. This implies that $u_s = 1$, so that $h_{\mu_0^{\pm}} = 0$, which is clearly positive.

Therefore, the ground state of the classical Hamiltonian is doubly degenerate and can be given by the Dirac measures $\mu_0^{\pm}$. □

Since the set of ground states $S_\infty(C_0(\mathbb{R}^2))$ is a compact convex subset of the total state space $S(C_0(\mathbb{R}^2))$, it follows from the previous lemma that

$$S_\infty(C_0(\mathbb{R}^2)) = \{\alpha\mu_0^+ + \beta\mu_0^-|\ \alpha + \beta = 1, \alpha, \beta \geqslant 0\}. \tag{2.99}$$

The extreme boundary is then clearly given by $\partial_e S_\infty(C_0(\mathbb{R}^2)) = \{\mu_0^+, \mu_0^-\}$. Then, on the one hand we have

$$\mu_0^{\pm}(\gamma_{-1}(f)) = \int_{\mathbb{R}^2} d\mu_0^{\pm} f(-x,-y)dxdy = f(0,\mp a), \tag{2.100}$$

but on the other hand, $\mu_0^{\pm}(f) = f(0,\pm a)$, which is clearly not equal to $f(0,\mp a)$ as $a > 0$.
Hence we conclude that $\partial_e S_\infty(C_0(\mathbb{R}^2))^G = \varnothing$, i.e. the $\mathbb{Z}_2$-symmetry is spontaneously broken.

[10] In general, for $A = C_0(X)$, pure states are given by $\omega_{x_0}(f) = f(x_0)$. Therefore, $H_{\omega_{x_0}} \simeq C_0(X)/C_0(X; x_0) \simeq \mathbb{C}$ via $[f] \mapsto f(y)$. Then, $\pi_{\omega_0}(f) = f(y)$ as operator $\mathbb{C} \to \mathbb{C}$.

Chapter 3

Curie-Weiss model

We will look at the quantum Curie-Weiss Hamiltonian, being an operator on the Hilbert space $\mathcal{H}_N \simeq \otimes_{x=1}^{N} \mathbb{C}^2$. It is extremely difficult to diagonalize this operator by hand and express its eigenvectors and eigenvalues by a formula in terms of N. Since for $N = 12$ the matrix representation of this operator will be already a 2^{12} dimensional matrix, even for a computer the diagonalization process will not be possible anymore when N increases too much. In particular, the ground state cannot be computed for say $N = 100$. Initially, this is a problem, because we want to say something about the convergence of the ground state in the limit $N \to \infty$ as we shall see in Chapter 6. However, we will see in this section that the ground state of the quantum Curie-Weiss Hamiltonian lies in a subspace of dimension $N + 1$. Thus, we may diagonalize this N-dependent operator with respect to a basis for this subspace. We will derive an expression for the matrix entries for this 'compressed' operator. Unfortunately, it still remains extremely difficult to prove an explicit N-dependent formula for the ground state eigenvector or eigenvalue. Nonetheless, simulations can now be made, easily up to $N = 5000$. This will be a great advantage, since this allows us to diagonalize this matrix for much larger N, so that we can get really an idea of the behaviour of the ground state. Moreover, as we will see in Chapters 4 and 6, these simulations also lead us to the connection with a Schrödinger operator and to the convergence of the ground state in the classical limit.

3.1 Properties of the Curie-Weiss model

Consider the Hamiltonian for the quantum Curie-Weiss model for ferromagnetism [22, p. 409], [6], [18]:

$$h_{\Lambda_N}^{\mathrm{CW}} = -\frac{J}{2|\Lambda_N|} \sum_{x,y \in \Lambda_N} \sigma_3(x)\sigma_3(y) - B \sum_{x \in \Lambda_N} \sigma_1(x), \tag{3.1}$$

where Λ_N is an arbitrary finite subset of $\mathbb{Z}^d$, $J > 0$ scales the spin-spin coupling, and B is an external magnetic field. This model describes a chain of N spin-1/2 particles with ferromagnetic coupling in a transverse magnetic field. In contrast to the quantum Ising model, the dimension of this model does not influence the behaviour. This follows from the fact that with

$$S_i^{\Lambda_N} = \frac{1}{|\Lambda_N|} \sum_{x \in \Lambda_N} \sigma_i(x), \tag{3.2}$$

we can write the Hamiltonian (3.1) as

$$h_{\Lambda_N}^{\mathrm{CW}} = -|\Lambda_N| \left(\frac{J}{2} (S_3^{\Lambda_N})^2 + B S_1^{\Lambda_N} \right). \tag{3.3}$$

The Hamiltonian acts on the Hilbert space $\mathcal{H}_{\Lambda_N} = \otimes_{x\in\Lambda_N} H_x$, where $H_x = \mathbb{C}^2$. The operator $\sigma_i(x)$ acts as the Pauli matrix σ_i on H_x and acts as the unit matrix $\mathbb{1}_2$ elsewhere. The local Hamiltonians $h_N \equiv h^{\mathrm{CW}}_{\Lambda_N}$ define a time evolution on the C^*-algebras

$$A_N \equiv A_{\Lambda_N} = B(\mathcal{H}_{\Lambda_N}) = \otimes_{x\in\Lambda_N} M_2(\mathbb{C}) \tag{3.4}$$

given by

$$\alpha^{(N)}_t(a_N) = \exp(ith_N)a_N \exp(-ith_N). \tag{3.5}$$

In contrast to the quantum Ising model, it can be shown [22, sec. 10.8] that (3.5) does not define a time evolution on the quasi-local C^*-algebra

$$A = \overline{\bigcup_{N\in\mathbb{N}} A_N} = \bigotimes_{x\in\mathbb{Z}} B(H_x), \tag{3.6}$$

since the Hamiltonian is not of short range, in that there does not exist a natural number $r \in \mathbb{N}$ such that $\Phi(X) \neq 0$ only if $|x - y| \leqslant r$ for all $x, y \in X$, where $X \subset \Lambda$. However, it turns out that it does define a time evolution on the commutative C^*-algebra

$$A^{(c)}_0 = C(S(M_n(\mathbb{C}))). \tag{3.7}$$

The Curie-Weiss chain has a $\mathbb{Z}_2$-symmetry given by 180-degree rotation about the x-axis, locally implemented by the unitary operator $u(x) = \sigma_1(x)$, which at each $x \in \Lambda_N$ yields $(\sigma_1, \sigma_2, \sigma_3) \mapsto (\sigma_1, -\sigma_2, -\sigma_3)$, since the unitary operator $u(x) = \sigma_1(x)$ satisfies $\sigma_1\sigma_j\sigma_1^* = -\sigma_j$ for $j \neq 1$. This symmetry is implemented by the unitary operator $u^{(N)}$ on $\mathcal{H}_N$ defined by

$$u^{(N)} = \otimes_{x\in\Lambda_N} \sigma_1(x). \tag{3.8}$$

It is not difficult to check that the relation $[h_N, u^{(N)}] = 0$ or $u^{(N)}h_N(u^{(N)})^* = h_N$, holds. The ensuing $\mathbb{Z}_2$-symmetry is then given by the automorphism $\gamma^{(N)}$ on A_N defined by

$$\gamma^{(N)}(a) = u^{(N)}a(u^{(N)})^* \quad (a \in A_N). \tag{3.9}$$

Since the Hamiltonian h_N commutes with $u^{(N)}$, we (locally) have

$$\alpha^{(N)}_t \circ \gamma^{(N)} = \gamma^{(N)} \circ \alpha^{(N)}_t. \tag{3.10}$$

Since $\gamma^2 = \mathrm{id}_{A_N}$, we have an action of the group $\mathbb{Z}_2 \cong \{\pm 1\}$ on A_N, where the nontrivial (i.e., $g = -1$) is sent to γ and the identity element (i.e., $g = 1$) to the identity id_{A_N}. By (3.10) this group acts on the set of ground states $S_0(A_N)$ of A_N relative to the dynamics $\alpha^{(N)}$. These results can also be found in [22, Chapter 10].

Corollary 10.23 from [22, p.411] discusses the classical dynamics on the Poisson manifold $S(M_n(\mathbb{C}))$, being the limit of the local Heisenberg dynamics $\alpha^{(N)}_t$ on A_N. In Chapter 6 we will give the analog of the $\mathbb{Z}_2$-action on this manifold for $n = 2$. But for now, we only focus on the local algebras $A_{\Lambda_N} = B(H_{\Lambda_N})$.

In this thesis, we only consider the case that $d = 1$, with $|\Lambda_N| = N$. We can apply the Perron-Frobenius theorem to equation (3.1) and find that for $B > 0$ each quantum mechanical Hamiltonian h_N has a unique ground state $\psi^{(0)}_N$ (see §5.3 for details). The local Hamiltonians h_N commute with the Symmetrizer operator, as we will see soon. Therefore, each h_N is permutation

invariant. Together with uniqueness, this implies that $\psi_N^{(0)}$ must share the invariance of h_N under permutations. Hence

$$\psi_N^{(0)} = \sum_{n_+=0}^{N} c(n_+/N)|n_+, n_-\rangle, \tag{3.11}$$

where $|n+, n_-\rangle$ is the totally symmetrized unit vector in $\otimes_{n=1}^N \mathbb{C}^2$, with n^+ spins up and $n_- = N - n_+$ spins down, and $c : \{0, 1/N, 2/N, ..., (N-1)/N, 1\} \to [0, 1]$ is some function such that $\sum_{n_+} c^2(n_+/N) = 1$, and $c(n_+/N) = c(n_-/N)$.
For $N < \infty$, and $B > 0$, one can show that the ground state $\psi_N^{(0)}$ is $\mathbb{Z}_2$-invariant, since the Curie-Weiss Hamiltonian commutes with $u^{(N)}$ and the ground state is unique. We will give a more detailed explanation in Chapter 7. For $N = \infty$ and $0 < B < 1$, the model has a doubly degenerate ground state that breaks the $\mathbb{Z}_2$-symmetry [22, Sec. 10.8] . A more precise analysis will be given in Chapter 6. This result is also known for the quantum Ising model [22, Thm. 10.11].

In the remaining part of this section, we reproduce the function c numerically using MATLAB and study its behaviour as N increases. In order to do this, we again take a glance to the Hamiltonian (3.1). Note that implicitly, with respect to the standard basis for $\mathcal{H}_{\Lambda_N} = \otimes_{n=1}^N \mathbb{C}^2$, this Hamiltonian is represented as a matrix since the spin Pauli matrices are represented in the standard basis for $\mathbb{C}^2$. We denote this standard basis, consisting of 2^N vectors, by β. Recall from linear algebra that $\beta = \{e_{n_1} \otimes e_{n_2} \otimes ... \otimes e_{n_N}\}_{n_1,...,n_N=1}^2$.

Consider the Symmetrizer operator S, defined as the projection onto the space of all totally symmetric vectors. Thus, S is given by

$$S(v) = \frac{1}{N!} \sum_{\sigma \in S_n} L_\sigma(v), \tag{3.12}$$

where v is a vector in the N-fold tensor product and the linear operator L_σ acts on $v \in \bigotimes_{n=1}^N \mathbb{C}^2$ by permuting the factors of v, thus $v_1 \otimes \cdot \cdot \cdot \otimes v_n \mapsto v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(n)}$. This operator is unitary extended by linearity since $L_\sigma^{-1} = L_\sigma^* = L_{\sigma^{-1}}$.

A basis for the space of totally symmetric vectors is given by the vectors $\{|n_+, n_-\rangle|\ n_+ = 0, ..., N,\ \ n_+ + n_- = N\}$, which spans a subspace. We denote this subspace by $\mathrm{Sym}^N(\mathbb{C}^2)$. If we write S with respect to the standard basis for the N-fold tensor product $\mathcal{H}_{\Lambda_N}$, denoted by $[S]_\beta$, and then project onto the basis vectors of the subspace $\mathrm{Sym}^N(\mathbb{C}^2)$, it follows that in the basis for $\mathrm{Sym}^N(\mathbb{C}^2)$, S is the identity matrix. Hence by computing $\langle n_+, n_-|[S]_\beta n'_+, n'_-\rangle$, we just transform the matrix representation of S with respect to β, to the matrix representation of S relative to the basis vectors $|n_+, n_-\rangle$ for $\mathrm{Sym}^N(\mathbb{C}^2)$. Since S acts as the identity operator on its range that is just $\mathrm{Sym}^n(\mathbb{C}^2)$, indeed the operator S written relative to the basis for $\mathrm{Sym}^N(\mathbb{C}^2)$ equals the identity matrix.

It is easy to see that the Hamiltonian (3.1) commutes with this action, i.e., $[h_N^{\mathrm{CW}}, L_\sigma] = 0$ for all $\sigma \in S_n$. Then S also commutes with h_N^{CW}. As S acts as the identity on $\mathrm{Sym}^N(\mathbb{C}^2)$, this subspace is invariant for S, and hence also for h_N^{CW}. We argue that the ground state $\psi_N^{(0)}$ of h_N^{CW} lies in $\mathrm{ran}(S) = \mathrm{Sym}^N(\mathbb{C}^2)$. If this is not the case, then there would exists an element $\sigma_j \in S_n$ such that $L_{\sigma_j}\psi_N^{(0)} \neq \psi_N^{(0)}$. Moreover, $L_{\sigma_j}\psi_N^{(0)}$ cannot be a scalar multiple of $\psi_N^{(0)}$, since it is permuted. Then $L_{\sigma_j}\psi_N^{(0)}$ would also be a ground state, since $h_N^{CW} L_{\sigma_j}\psi_N^{(0)} = L_{\sigma_j} h_N^{CW}\psi_N^{(0)} = \epsilon_0 L_{\sigma_j}\psi_N^{(0)}$, for some number ϵ_0. By uniqueness, the above implies that $L_{\sigma_j}\psi_N^{(0)} = z_{\sigma_j}\psi_N^{(0)}$, for some $|z_{\sigma_j}| = 1$. This is a contradiction.

Hence, the ground state lies in the linear span of eigenfunctions of S, and we may indeed write (3.11). Therefore, we can determine the coefficients of $\psi_N^{(0)}$ using this subspace by diagonalizing the compressed $(N+1)\times(N+1)$-matrix instead of the original $2^N \times 2^N$-matrix. We can derive a specific form of the matrix representation of h_N^{CW} with respect to the basis $|n_+, n_-\rangle$ for $\mathrm{Sym}^n(\mathbb{C}^2)$. This will be given in the following theorem.

Theorem 3.1. *In the basis* $\{|n_+, n_-\rangle \mid n_+ = 0, 1, ..., N, \quad n_+ + n_- = N\}$*, the Hamiltonian* (3.1) *is a tridiagonal matrix of dimension* $N+1$ *given by*

$$-\frac{J}{2|\Lambda_N|}(n_+ - n_-)^2 \quad \textit{on the diagonal,} \tag{3.13}$$

$$-B\sqrt{n_-(n_+ + 1)} \quad \textit{on the upper diagonal,} \tag{3.14}$$

$$-B\sqrt{(n_- + 1)n_+} \quad \textit{on the lower diagonal.} \tag{3.15}$$

Proof. As we have seen above, there are $N+1$ linearly independent totally symmetric basis vectors, i.e., the subspace $\mathrm{Sym}^N(\mathbb{C}^2)$ is $(N+1)$-dimensional and there are 2^N standard basis vectors β_i spanning the the space $\mathcal{H}_{\Lambda_N}$. Since each basis vector $\beta_i \in \beta$ consists of tensor products of e_1 and e_2, we know that there are $\binom{N}{k}$ basis vectors of β with k times the vector e_2 and hence $(N-k)$-times the vector e_1. This shows that we have a partition of β, and hence $N+1$ orbits $\mathscr{O}^k$. Each orbit $\mathscr{O}^k$ consists of $\binom{N}{k}$-basis vectors β_i with the same number of occurrence of the vectors e_2 and e_1. Therefore, we have a bijection between the number of orbits and the dimension of $\mathrm{Sym}^N(\mathbb{C}^2)$. The correspondence is made as follows:

$$\mathscr{O}^k \leftrightarrow |N-k, k\rangle. \tag{3.16}$$

Here k in $|N-k, k\rangle$ labels the number of occurrence of the vector e_2 in any of the basis vectors $\beta_i \in \beta$, and $N-k$ in $|N-k, k\rangle$ labels the occurrence of the vector e_1 in β_i. Hence, $N-k$ stands for the number n_+ of spins in the up direction, whilst the second position $k = n_-$ denotes the number of down spins.

Consider now such a symmetric basis vector $|n_+, n_-\rangle$. Using (3.12), it is not difficult to show that

$$|n_+, n_-\rangle = \frac{1}{\sqrt{\binom{N}{n_+}}} \sum_{l=1}^{\binom{N}{n_+}} \beta_{n_+,l}, \tag{3.17}$$

where the subindex l in $\beta_{n_+,l}$ labels the basis vector $\beta_{n_+,l} \in \beta$ within the same orbit $\mathscr{O}^{n_+}$. Since we have $\binom{N}{n_+}$ such vectors per orbit, the sum in the above equation indeed is from $l = 1, ..., \binom{N}{n_+}$.

Now given two arbitrary vectors $|n_+, n_-\rangle$ and $|n'_+, n'_-\rangle$, then in order to prove the theorem, we have to compute the expression

$$\langle n_+, n_-|h_N^{\mathrm{CW}}|n'_+ n'_-\rangle, \quad (n_+, n'_+ = 0, ..., N) \tag{3.18}$$

In the above expression we have used the well-known bra-ket notation. Hence, we have to compute

$$\frac{1}{\sqrt{\binom{N}{n_+}}}\frac{1}{\sqrt{\binom{N}{n'_+}}} \sum_{l=1}^{\binom{N}{n_+}} \sum_{k=1}^{\binom{N}{n'_+}} \langle \beta_{n_+,l}|h_N^{\mathrm{CW}}|\beta_{n'_+,k}\rangle \quad (n_+, n'_+ = 0, ..., N) \tag{3.19}$$

By linearity, we may compute this for

$$h_N^{(1)} = \sum_{x,y=1}^{N} \sigma_3(x)\sigma_3(y) = (\sum_{x=1}^{N} \sigma_3(x))(\sum_{y=1}^{N} \sigma_3(y)), \quad \text{and}$$
$$h_N^{(2)} = \sum_{x=1}^{N} \sigma_1(x) \tag{3.20}$$

separately. Note that

$$\begin{aligned}
&\sigma_3 e_1 = e_1, \\
&\sigma_3 e_2 = -e_2, , \\
&\sigma_1 e_1 = e_2, , \\
&\sigma_1 e_2 = e_1.
\end{aligned} \tag{3.21}$$

Fix N and n_+, and put

$$\begin{aligned}
W_{n_+}^1 &= \{y \in \{1, ..., N\} |\ \beta_{n_+} \text{ has } e_1 \text{ on position } y\ \}, \quad \text{and} \\
W_{n_+}^2 &= \{y \in \{1, ..., N\} |\ \beta_{n_+} \text{ has } e_2 \text{ on position } y\ \}.
\end{aligned} \tag{3.22}$$

Then

$$\#W_{n_+}^1 + \#W_{n_+}^2 = n_+ + (N - n_+) = n_+ + n_- = N. \tag{3.23}$$

Both sets are clearly disjoint. We use this for the next computation. We start with $h_N^{(1)}$. Then we compute

$$\begin{aligned}
&\frac{1}{\sqrt{\binom{N}{n_+}}} \frac{1}{\sqrt{\binom{N}{n'_+}}} \sum_{l=1}^{\binom{N}{n_+}} \sum_{k=1}^{\binom{N}{n'_+}} \langle \beta_{n_+,l} | h_N^{(1)} | \beta_{n'_+,k} \rangle = \\
&\frac{1}{\sqrt{\binom{N}{n_+}}} \frac{1}{\sqrt{\binom{N}{n'_+}}} \sum_{l=1}^{\binom{N}{n_+}} \sum_{k=1}^{\binom{N}{n'_+}} \langle \beta_{n_+,l} | \Big(\sum_{x=1}^{N} \sigma_3(x) \Big) \Big(\sum_{y=1}^{N} \sigma_3(y) \Big) | \beta_{n'_+,k} \rangle = \\
&\frac{1}{\sqrt{\binom{N}{n_+}}} \frac{1}{\sqrt{\binom{N}{n'_+}}} \sum_{l=1}^{\binom{N}{n_+}} \sum_{k=1}^{\binom{N}{n'_+}} \langle \beta_{n_+,l} | \Big(\sum_{x \in W_{n'_+}^1} + \sum_{x \in W_{n'_+}^2} \sigma_3(x) \Big) \Big(\sum_{y \in W_{n'_+}^1} + \sum_{y \in W_{n'_+}^2} \sigma_3(y) \Big) | \beta_{n'_+,k} \rangle = \\
&\frac{1}{\sqrt{\binom{N}{n_+}}} \frac{1}{\sqrt{\binom{N}{n'_+}}} \sum_{l=1}^{\binom{N}{n_+}} \sum_{k=1}^{\binom{N}{n'_+}} (n'_+ - n'_-)^2 \langle \beta_{n_+,l} | \beta_{n'_+,k} \rangle = \\
&(n'_+ - n'_-)^2 \langle n_+, n_- | n'_+, n'_- \rangle = \\
&(n'_+ - n'_-)^2 \delta_{n_+,n'_+} \delta_{n_-,n'_-}.
\end{aligned} \tag{3.24}$$

Here, we used the fact that the vectors $|n_+, n_-\rangle$ form a orthonormal basis for $\mathrm{Sym}^N(\mathbb{C}^2)$. Hence, the matrix entries of $h_N^{(1)}$ represented with respect to the $|n_+, n_-\rangle$-vectors are given by $(n'_+ - n'_-)^2$ on the diagonal.

We compute the second term $h_N^{(2)}$ in a similar way:

$$\frac{1}{\sqrt{\binom{N}{n_+}}}\frac{1}{\sqrt{\binom{N}{n'_+}}}\sum_{l=1}^{\binom{N}{n_+}}\sum_{k=1}^{\binom{N}{n'_+}}\langle\beta_{n_+,l}|h_N^{(2)}|\beta_{n'_+,k}\rangle =$$

$$\frac{1}{\sqrt{\binom{N}{n_+}}}\frac{1}{\sqrt{\binom{N}{n'_+}}}\sum_{l=1}^{\binom{N}{n_+}}\sum_{k=1}^{\binom{N}{n'_+}}\langle\beta_{n_+,l}|\sum_{x=1}^{N}\sigma_1(x)|\beta_{n'_+,k}\rangle =$$

$$\frac{1}{\sqrt{\binom{N}{n_+}}}\frac{1}{\sqrt{\binom{N}{n'_+}}}\sum_{l=1}^{\binom{N}{n_+}}\sum_{k=1}^{\binom{N}{n'_+}}\langle\beta_{n_+,l}|\Big(\sum_{x\in W^1_{n'_+}}+\sum_{x\in W^2_{n'_+}}\sigma_1(x)\Big)|\beta_{n'_+,k}\rangle =$$

$$\frac{1}{\sqrt{\binom{N}{n_+}}}\frac{1}{\sqrt{\binom{N}{n'_+}}}\Big(\binom{N}{n_+}n_-\langle\beta_{n_+,l}|\beta_{n'_+-1,k}\rangle+\binom{N}{n_-}n_+\langle\beta_{n_+,l}|\beta_{n'_++1,k}\rangle\Big) =$$

$$\sqrt{n_-(n_++1)}\delta_{n_+,n'_+-1}+\sqrt{n_+(n_-+1)}\delta_{n_+,n'_++1}. \tag{3.25}$$

We used the fact that the vectors $\beta_{n'_+,l}$ are orthonormal, that

$$\frac{1}{\sqrt{\binom{N}{n_+}}}\frac{1}{\sqrt{\binom{N}{n'_+}}}\binom{N}{n_+}n_- = \sqrt{n_-(n_++1)}, \tag{3.26}$$

with $n'_+ - 1 = n_+$, and that

$$\frac{1}{\sqrt{\binom{N}{n_+}}}\frac{1}{\sqrt{\binom{N}{n'_+}}}\binom{N}{n_-}n_+ = \sqrt{n_+(n_-+1)}, \tag{3.27}$$

, with $n'_+ + 1 = n_+$. Hence the matrix entries of $h_N^{(2)}$ written with respect to the symmetric basis vectors $|n_+, n_-\rangle$, are given by $\sqrt{n_-(n_++1)}$ on the upper diagonal and by $\sqrt{n_+(n_-+1)}$ on the lower diagonal.

We conclude that the Hamiltonian with respect to this basis is a tridiagonal matrix with the desired entries. □

3.2 Numerical simulations

We have seen that the ground state of the N-dependent Curie-Weiss Hamiltonian h_N^{CW} lies in the symmetric subspace $\mathrm{Sym}^N(\mathbb{C}^2)$. This followed from a one line proof using the fact that h_N^{CW} commutes with the Symmetrizer operator S, and that the ground state of h_N^{CW} is unique, which we will prove in Chapter 5. As a result, we could diagonalize the operator originally defined on $\bigotimes_{n=1}^N \mathbb{C}^2$, with respect to a basis for $\mathrm{Sym}^N(\mathbb{C}^2)$, which we have taken to be the canonical one. In the previous paragraph, we have showed an explicit formula for the matrix entries of the operator h_N^{CW} represented with respect to this basis. In Chapter 4, we will argue that for $0 < B < 1$ this $(N+1)$-dimensional matrix, which we denote by J_{N+1}, can be linked to a Schrödinger operator with a symmetric double well on $L^2([0,1])$, for N sufficiently large, but finite. This will be one of the most important results in this thesis. Since it is known [37], [14] that for a sufficiently high and broad enough potential barrier the ground state of such a Schrödinger operator is approximately given by two Gaussians, each of them located in one of the wells of the potential, we might expect the

same result for J_{N+1}, for these values of N. In fact, the first two eigenfunctions of this Schrödinger operator are approximately given by

$$\begin{aligned} \psi^{(0)} &\cong \frac{T_a(\varphi_0) + T_{-a}(\varphi_0)}{\sqrt{2}}; \\ \psi^{(1)} &\cong \frac{T_a(\varphi_0) - T_{-a}(\varphi_0)}{\sqrt{2}}. \end{aligned} \tag{3.28}$$

Here, $T_{\pm a}$ is the translation operator over distance a (i.e., $(T_{\pm a}\varphi_0)(x) = \varphi_0(x \pm a)$), where $\pm a$ denotes the minima of the potential well. The functions φ_n are the weighted Hermite polynomials given by $\varphi_n(x) = e^{-x^2/2}H_n(x)$, with H_n the Hermite polynomials. We diagonalized the operator J_{N+1} and plotted the first two (discrete) eigenfunctions $\psi_N^{(0)}$ and $\psi_N^{(1)}$. For convenience, we scaled the grid to unity. (See Figure 3.1 and 3.2).

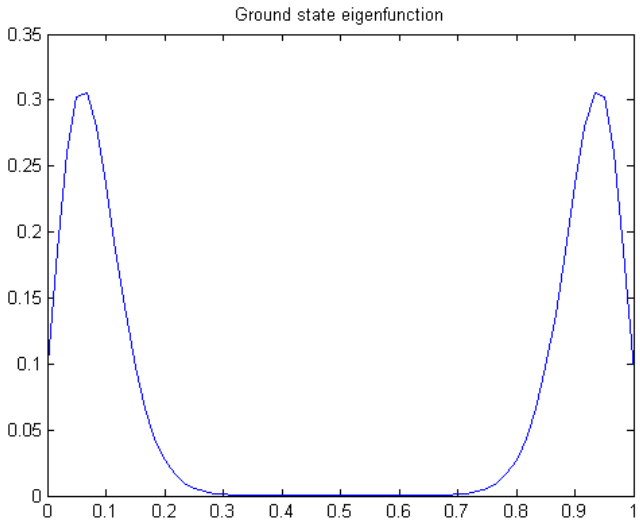

Figure 3.1: The ground state eigenfunction of h_N^{CW}, computed from the tridiagonal matrix J_{N+1} for $N = 60$, $J = 1$ and $B = 1/2$.

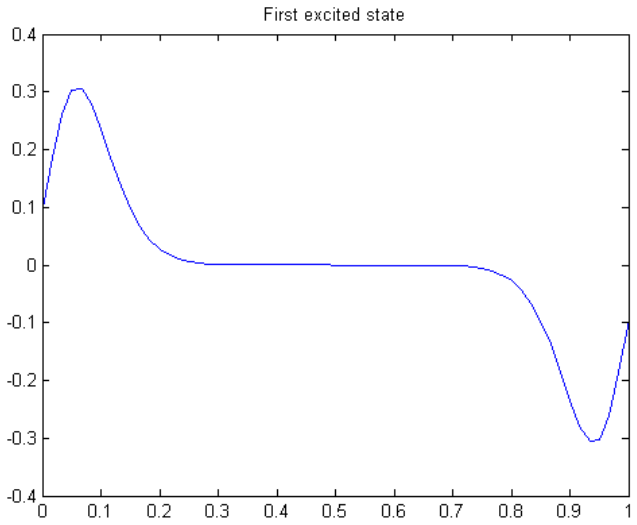

Figure 3.2: The first excited state of h_N^{CW}, computed from the tridiagonal matrix J_{N+1} for $N = 60$, $J = 1$ and $B = 1/2$.

From the above two plots, it is quite clear that both eigenvectors of h_N^{CW} are approximately given by (3.28). However, one has to beware of the following fact: since we do not know if the first excited state is unique, it might happen that it does not lie in $\mathrm{Sym}^N(\mathbb{C}^2)$. As a result, it could happen that the first excited state computed from the tridiagonal matrix J_{N+1}, is not the same as the one from the original Hamiltonian h_N^{CW}, and then Figure 3.2 does not make any sense. Fortunately, we have shown numerically up to $N = 12$, that the first excited state of h_N^{CW} represented as a matrix on the space $\mathbb{C}^{2^N}$ is indeed the same as the one corresponding to the tridiagonal matrix J_{N+1}. Unfortunately, we could not check this for larger N due to the limited power of the computer.

In Chapter 4, we will see that for $0 < B < 1$ each of the two peaks of the ground state eigenvector of the N-dependent Curie-Weiss Hamiltonian is indeed located in one of the wells of some symmetric potential. However, due to numerical degeneracy of the ground state $\psi_N^{(0)}$ and first excited state $\psi_N^{(1)}$ for about $N \geqslant 80$, these two states will form a linear combination, even though mathematically the ground state is unique for any finite N. Assuming that $\psi_N^{(1)}$ is indeed in $\mathrm{Sym}^N(\mathbb{C}^2)$, then for these relative large values of N, the new (numerical) degenerate ground state eigenvector is given by the functions

$$\begin{aligned} \chi_+ &= \frac{\psi_N^{(0)} + \psi_N^{(1)}}{\sqrt{2}}; \\ \chi_- &= \frac{\psi_N^{(0)} - \psi_N^{(1)}}{\sqrt{2}}. \end{aligned} \tag{3.29}$$

Using this result and equation (3.28), it follows by a simple calculation that

$$\begin{aligned} \chi_+ &\cong T_a\varphi_0; \\ \chi_- &\cong T_{-a}\varphi_0. \end{aligned} \tag{3.30}$$

Of course, the functions $\varphi_n(x)$ now have to be understood as functions on a discrete grid. This is also exactly what we observe for the values $N \geqslant 80$: plotting the ground state and the first excited state of h_N^{CW} ($B = 1/2$ and $J = 1$) gives a Gaussian shaped curve, each located in one of the

wells. For $N = 60 < 80$, we have seen in Figure 3.1 above that the ground state is doubly peaked and therefore given by $\psi_N^{(0)}$, rather than χ_+. This makes sense, since the energy levels are not yet degenerate even for the computer.

Chapter 4

Curie-Weiss model as a discretized Schrödinger operator

In the limit $N \to \infty$, the ground state of the local Curie-Weiss Hamiltonians h_N^{CW} from (3.1), defined on $\bigotimes_{n=1}^{N} \mathbb{C}^2$ can be linked to the minima of a classical function h_∞^{CW}, defined by (1.5), on the commutative C^*-algebra $C(B^3)$, with $B^3 \subset \mathbb{R}^3$ the closed unit ball. This is based on the idea of *deformation quantization*, which we will explain in Chapter 6. It is, however, not well understood how the *operators* h_N^{CW} itself converge to the function h_∞^{CW} when $N \to \infty$, only convergence of the ground state is understood[1]. However, the Curie-Weiss model can also be linked to a specific Schrödinger operator. This will be the topic of this chapter. For this, we consider the Curie-Weiss Hamiltonian, restricted to the symmetric subspace $\mathrm{Sym}^N(\mathbb{C}^2)$. Representing this operator with respect to the canonical basis $|n_+, n_-\rangle$ for this subspace yielded a $N+1$-dimensional matrix. If we denote this matrix by J_{N+1}, then it is also not so clear if the limit $\lim_{N\to\infty} J_{N+1}$ exists, since all entries are unbounded in N. When we scale this operator by N, it is easy to see that the entries of J_{N+1}/N are bounded. We will see in §4.6 that this scaled operator corresponds to a matrix representing a discretization of a Schrödinger operator, where the dimension of this matrix also depends on the same N. The spectral properties of J_{N+1}/N and the discretization matrix will become more similar when N gets larger. However, as we will see, the connection with this Schrödinger operator makes sense, only for finite N, since for $N = \infty$, the Schrödinger operator is not defined. Nonetheless, we will see in §6.3 that in the limit $N \to \infty$ (read: $\hbar = 1/N \to 0$), the ground state eigenfunction of this Schrödinger operator converges to some Dirac measure, corresponding to the minima of a classical function on the commutative C^*-algebra $C([0,1] \times \mathbb{R})$. This is again based on deformation quantization, as explained in Appendix E or [22, Sec. 10.1].

In the first paragraph we mention some general facts about the diagonalization of the N-dependent Curie-Weiss Hamiltonian, written with respect to the canonical basis $|n_+, n_-\rangle$ for the symmetric subspace $\mathrm{Sym}^N(\mathbb{C}^2)$. Then we show that the spectrum of J_{N+1} contains $N+1$ distinct eigenvalues. The next step is to give an idea of a possible proof showing that for finite, but large N, the spectrum of this 'compressed' Curie-Weiss Hamiltonian becomes approximately twofold degenerate. In §4.4 we show that the Hamiltonian is 'almost' linked to a classical orthogonal polynomial (since for increasing N we observe numerically that the eigenvectors behave like weighted Hermite polynomials, one might expect that for these values of N some classical orthogonal polynomials would play a role.)
The next three paragraphs together explain how the operator J_{N+1}/N can be related to a Schrödinger operator with a symmetric double well potential. For this double well, which is the basis for SSB in the classical limit, we need $B \in [0, 1)$. For convenience, we take $B = 1/2$.

[1] The dynamics of h_N^{CW}, however, does converge to the classical dynamics of h_∞^{CW} (See e.g. [22, Cor. 10.23]).

In the last paragraph, we use the semiclassical WKB approximation in order to compute the so-called energy splittings for the symmetric double well potential. The goal is to compare the energy levels obtained from the matrix J_{N+1}/N to those of the Schrödinger operator analog in the semiclassical limit i.e., for large but finite N. In a naive way, when the barrier of the potential is sufficiently high and broad, the double well could be seen as a pair of decoupled harmonic oscillators. In this case the ground state is doubly degenerate and tunneling is not allowed, i.e., in the classical limit. However, in a semi-classical approximation, the particle can tunnel through the barrier in the middle. This breaks the degeneracy and brings out the first excited state, with a slightly higher energy than the ground state. The energy difference between both levels is known as the ground state energy splitting. For an $\hbar$-dependent Schrödinger operator, this energy splitting depends on $\hbar$. In our case, $\hbar$ plays the role of $1/N$. We will derive a formula for this energy splitting applied to a double well potential that corresponds to a Schrödinger operator and that is extracted from our matrix J_{N+1}/N, all explained in §4.5 - §4.7.

4.1 Unfolding the eigenfunctions of the quantum Curie-Weiss Hamiltonian

Recall that the Hamiltonian for the Curie-Weiss-model on the N-fold tensor product of $\mathbb{C}^2$ is given by

$$h_N^{\mathrm{CW}} = -\frac{J}{2N}\sum_{x,y\in\Lambda_N}\sigma_3(x)\sigma_3(y) - B\sum_{x\in\Lambda}\sigma_1(x). \tag{4.1}$$

In order to find the ground state of the Hamiltonian, we have seen that we can represent our Hamiltonian with respect to the symmetric basis of $\mathrm{Sym}^N(\mathbb{C}^2)$, since the ground state lies in this subspace. This reduces the problem to an eigenvalue problem of an $(N+1)\times(N+1)$- matrix. In Theorem 3.1 we have deduced an explicit formula for the matrix representation of the Curie-Weiss Hamiltonian with respect to this symmetric basis. The crucial step is that the matrix represented in this basis is tridiagonal. As we will see later in this chapter, this gives also the link with the harmonic oscillator in a symmetric double well.

In order to compute the eigenvectors, we need to find the eigenvalues, which can be done by finding the zeros of its characteristic polynomial. Therefore, we need to compute the determinant of the matrix $h_N^{\mathrm{CW}} - \lambda_i I$, where I is the identity matrix and λ_i the scalar to be found. However, since we know that the ground state eigenvector lies in the symmetric subspace, it suffices to diagonalize the tridiagonal J_{N+1} with entries given by Theorem 3.1. Hence, denoting the ground state eigenvalue by λ_0 and using Theorem 3.1, it follows that:

$$J_{N+1}-\lambda_0 I = \begin{bmatrix} -\frac{J}{2N}(N-0)^2-\lambda_0 & -B\sqrt{N} & 0 & \dots & 0 \\ -B\sqrt{N} & -\frac{J}{2N}(N-2)^2-\lambda_0 & -B\sqrt{(N-1)(2)} & \dots & 0 \\ 0 & -B\sqrt{(N-1)(2)} & -\frac{J}{2N}(N-4)^2-\lambda_0 & \dots & 0 \\ 0 & 0 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \end{bmatrix}_{N+1} \tag{4.2}$$

We have to compute the determinant of this matrix and solve this for λ_0. We know from [26] that the determinant of an arbitrary tridiagonal matrix A is given by $\det(A) =$

$$\det\begin{bmatrix} a_1 & b_1 & \dots & 0 \\ c_1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & b_{n-1} \\ 0 & \dots & c_{n-1} & a_n \end{bmatrix} = \left[\begin{pmatrix} a_n & -b_{n-1}c_{n-1} \\ 1 & 0 \end{pmatrix}\cdots\begin{pmatrix} a_2 & -b_1c_1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a_1 & 0 \\ 1 & 0 \end{pmatrix}\right]_{11} \tag{4.3}$$

It can be verified that this determinant satisfies the recursion relation:

$$\begin{aligned} f_{n+1}(\lambda) &= (a_{n+1} - \lambda) f_n(\lambda) - b_n^2 f_{n-1}(\lambda) \\ f_1(\lambda) &= a_1 - \lambda \\ f_0(\lambda) &= 0. \end{aligned} \tag{4.4}$$

One can solve this recursion and find an expression for the determinant, i.e., for the characteristic polynomial. However in our case things get complicated. The restricted Hamiltonian J_{N+1} has entries that depend on N, and change when N changes. Consequently, we deal with a recursion relation with non-constant coefficients, which in general is hard to solve. Computer simulations have showed that most zeros of the characteristic polynomial are irrational. We did not succeed yet to give a general solution for the N-depending zeros of this determinant. In particular, the ground state energy cannot be exactly computed.
We can still get an idea of the way the N-dependent ground state eigenvector behaves. Of course, this is now a function of the corresponding eigenvalue λ_0. Applying the Gauss-Jordan algorithm, it is easy to see that the coefficients in the corresponding eigenvector can be written as a continued fraction of finite length that increases with increasing coefficient. The coefficients in the eigenvector are given below. We let

$$\begin{aligned} a_{n_+}^N &= -\frac{1}{2N}(n_+ - n_-)^2 - \lambda_0^N; \\ b_{n_+}^N &= -B\sqrt{(n_-(n_+ + 1))}, \end{aligned} \tag{4.5}$$

where n_+ runs from 0 to N, and $n_+ + n_- = N$. Then the coefficients $c_{n_+}^N$ in the eigenvector $c^N = (c_0^N, c_1^N, ..., c_N^N)$ are given by

$$\begin{aligned} c_0^N &= 1 \\ c_1^N &= -\frac{1}{b_0^N} a_0^N c_0 \\ c_2^N &= -\frac{1}{b_1^N}\left[a_1^N - \frac{(b_0^N)^2}{a_0^N}\right] c_1 \\ c_3^N &= -\frac{1}{b_2^N}\left[a_2^N - \frac{(b_1^N)^2}{a_1^N - \frac{(b_0^N)^2}{a_0^N}}\right] c_2 \\ c_4^N &= -\frac{1}{b_3^N}\left[a_3^N - \frac{(b_2^N)^2}{a_2^N - \frac{(b_1^N)^2}{a_1^N - \frac{(b_0^N)^2}{a_0^N}}}\right] c_3 \\ &\vdots \qquad\qquad\qquad\qquad \vdots \end{aligned} \quad ,$$

where the dots run to N. Since we have a free choice for c_0^N, we put $c_0^N = 1$. In particular, since the ground state is $\mathbb{Z}_2$-invariant we only need to compute the first $N/2$ equations for this eigenvector. Moreover, these coefficients and hence the eigenvector c^N still depend on the eigenvalue, which we do not exactly know. Even if we would know an analytic expression for the desired eigenvalue, it still would be extremely difficult to understand mathematically how these coefficients behave, especially if N increases, because the fraction increases with N. Furthermore, when we take the scaled operator J_{N+1}/N, its coefficients still depend on N, and it does not make computations much easier. Therefore, it is important to consider the behaviour of c^N rather than trying to compute all these coefficients analytically. This can be easily understood by computer simulations.

4.2 The spectrum

Fortunately, we can say something about the spectrum, which will be stated in the theorem below. The proof is based on [30].

Theorem 4.1. *The spectrum of the N- dependent Curie-Weiss Hamiltonian, written with respect to the symmetric basis $|n_+, n_-\rangle$ for the symmetric subspace $Sym^N(\mathbb{C}^2)$, consists of $N+1$ distinct eigenvalues.*

Proof. Recall that the Curie-Weiss Hamiltonian written in this basis is a $N+1$- dimensional tridiagonal matrix with entries $-B\sqrt{(N-n_+)(n_++1)}$, on the lower diagonal, $-\frac{J}{2N}(n_+-n_-)^2$ on the diagonal, and $-B\sqrt{(N-n_-)(n_-+1)}$ on the upper diagonal. Here, we fix $B=1/2$, and $J=1$. Again we denote this matrix by J_{N+1}. Since for every N the matrix J_{N+1} is of finite dimension, its spectrum is discrete, i.e. it consists of eigenvalues.
Observe that J_{N+1} is real and symmetric and that the lower diagonal and upper diagonal elements are non-zero. We show first that $\text{rank}(J_{N+1}) \geqslant N$.

We show that if $J_{N+1}v = 0$ has two non-trivial solutions, they are multiples of each other. Therefore, let $v, w \neq 0$ be two non-trivial solutions. Then we get the following $N+1$ equations for the vector components v_i of v:

$$a_1v_1 + b_1v_2 = 0, \tag{4.6}$$
$$b_iv_i + a_{i+1}v_{i+1} + b_iv_{i+2} = 0 \quad (i = 1, 2, ..., N-1), \tag{4.7}$$
$$b_Nv_N + a_{N+1}v_{N+1} = 0. \tag{4.8}$$

Similarly, we get such equations for w_i. From the first equation, we see that $v_2 = \frac{-a_1v_1}{b1}$, which exists, as $b_1 \neq 0$. Similarly, the next $N-1$ equations determine that $v_{i+2} = \frac{-b_iv_i - a_{i+1}v_{i+1}}{b_i}$, for $i = 1, 2, ..., N-1$. These equations determine the vector v, given the first component v_1. It also follows that if $v_1 = 0$, then $v = 0$. The same holds for w. By assumption, $v_1, w_1 \neq 0$. Define $c = \frac{w_1}{v_1}$. The first N equations for w_i yield $w_i = cv_i$, for $i = 1, ..., N+1$. Thus $w = cv$. We conclude that, if there are non trivial solutions, they are multiples of each other. This proves also that the dimension of the null space is at most one-dimensional and therefore, the rank is a least $N+1-1 = N$- dimensional.

Now let λ be an eigenvalue of J_{N+1}. This means that there exists a non-trivial solution v to the equation $(J_{N+1} - \lambda I)v = 0$. Since the matrix J_{N+1} is real symmetric, its eigenvalues are real, and therefore $J_{N+1} - \lambda I$ is also real symmetric with non zero lower and upper diagonal entries. It follows by the previous observation that the null space is at most one dimensional, and since λ is an eigenvalue, it is at least one-dimensional and thus one dimensional. Thus the geometric multiplicity of λ is one. In theory, it could be that its algebraic multiplicity of J_{N+1} is larger than one, but then the matrix is not diagonalizable. Since C is normal, it is diagonalizable, and therefore, its algebraic multiplicity is one as well. This holds for any eigenvalue. We conclude that J_{N+1} has $N+1$ distinct eigenvalues. □

The same result holds of course for the scaled operator J_{N+1}/N. This shows in particular that the ground state of this tridiagonal matrix is simple, and hence unique. (This is what we already know by the argumentation given in §3.1.) It also shows that if the excited states of h_N^{CW} are symmetric, i.e., they lie in the symmetric subspace, so that they can be found by diagonalizing J_{N+1}, then they are unique as well.

4.3 Degeneracy

The original Curie-Weiss Hamiltonian h_N^{CW} from Equation (3.1), defined on $\bigotimes_{n=1}^{N}\mathbb{C}^2$, does not converge to some operator on the quasi-local algebra $\bigotimes_{n=1}^{\infty}\mathbb{C}^2$. The compressed Curie-Weiss operator J_{N+1}, is of course an operator on an $(N+1)$-dimensional space. It is still not clear if $\lim_{N\to\infty} J_{N+1}$ exists, since all entries are unbounded in N. Nonetheless, for each finite N, the operator is well defined, and hence we can diagonalize it in order to obtain information about the spectrum and the eigenfunctions. We have already seen that the ground state of h_N^{CW} is symmetric, and can be found by diagonalizing J_{N+1}. Note that we do not know this result for the excited states.

In this paragraph we argue that for sufficiently large but finite N, the lowest eigenvalues of the spectrum of J_{N+1} and hence of J_{N+1}/N, become approximately two fold degenerate with a fixed energy splitting. Of course, these arguments are based on numerical computations. We have already deduced a formula for the characteristic equation of the operator J_{N+1}/N given by (4.4). We can rewrite this formula in a more suitable form. This will be given in the next theorem.

Theorem 4.2. *The characteristic polynomial of the scaled compressed Curie-Weiss Hamiltonian J_{N+1}/N is given by*

$$det\Big(J_{N+1}/N - \lambda\mathbf{1}\Big) \equiv p_{N+1}(\lambda) = p_{\frac{N}{2}}(\lambda)\Big(p_{\frac{N}{2}+1}(\lambda) - b_{N/2}^2 p_{\frac{N}{2}-1}(\lambda)\Big). \tag{4.9}$$

Here $p_{\frac{N}{2}}$ is the characteristic polynomial corresponding to the square matrix of dimension $N/2$ that forms the left upper block in the matrix J_{N+1}/N. Similarly, the characteristic polynomial $p_{\frac{N}{2}\pm 1}$ corresponds to the square matrix of dimension $N/2 \pm 1$ that forms the left upper block in J_{N+1}/N. The number $b_{N/2}$ denotes the off-diagonal element of J_{N+1}/N on position $N/2$.

Proof. The proof of this theorem is based on [36].
Assume for convenience that N is even. Put

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{4.10}$$

and

$$B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}. \tag{4.11}$$

Here A_{11} and B_{22} are square matrices of dimension $N/2$. A_{22} and B_{11} are matrices of dimension 1, and A_{12}, A_{21}, B_{12} and B_{21} are non-square matrices of dimension $1 \times N/2$ or $N/2 \times 1$. Now, we consider the following matrix of dimension $N/2 + N/2 + 1 = N + 1$:

$$D = \begin{bmatrix} A_{11} & A_{12} & 0 \\ A_{21} & A_{22} + B_{11} & 0 \\ 0 & B_{21} & B_{22} \end{bmatrix}. \tag{4.12}$$

This matrix is called the $1-$ subdirect sum of A and B, denoted by $D = A \oplus_1 B$. We write $a_{22} = A_{22}$ and $b_{11} = B_{11}$, to display that these are matrices of order 1×1.

We shall deduce a formula for the characteristic polynomial corresponding to D. The determinant

is a multilinear function of its columns, so we have

$$\det(D-\lambda\mathbf{1}) = \tag{4.13}$$
$$\tag{4.14}$$
$$\det\begin{bmatrix} A_{11}-\lambda\mathbf{1} & A_{12} & 0 \\ A_{21} & a_{22}+b_{11}-\lambda\mathbf{1} & B_{12} \\ 0 & B_{21} & B_{22}-\lambda\mathbf{1}\end{bmatrix} = \tag{4.15}$$
$$\tag{4.16}$$
$$\det\begin{bmatrix} A_{11}-\lambda\mathbf{1} & A_{12} & 0 \\ A_{21} & a_{22}-\lambda\mathbf{1} & 0 \\ 0 & B_{21} & B_{22}-\lambda\mathbf{1}\end{bmatrix} + \det\begin{bmatrix} A_{11}-\lambda\mathbf{1} & A_{12} & 0 \\ A_{21} & b_{11} & B_{12} \\ 0 & B_{21} & B_{22}-\lambda\mathbf{1}\end{bmatrix}. \tag{4.17}$$

This leads to

$$\det(D-\lambda\mathbf{1}) = \tag{4.18}$$
$$\det(A-\lambda\mathbf{1})\det(B_{22}-\lambda\mathbf{1})+ \tag{4.19}$$
$$\det(A_{11}-\lambda\mathbf{1})\det\begin{bmatrix} b_{11} & B_{12} \\ B_{21} & B_{22}-\lambda\mathbf{1}\end{bmatrix}. \tag{4.20}$$

We apply this result to our matrix tridiagonal matrix J_{N+1}/N.

It follows that $a_{22} = b_{11} = 0, A_{11} = B_{22} \in M_{\frac{N}{2}}(\mathbb{R})$, and $A_{21} = A_{12} = B_{12} = B_{21}$ are the $(N/2\times 1)$- matrices with on the last entry the element $-B\sqrt{(1-1/2)(1/2+1/N)}$. It follows that

$$\det(J_{N+1}/N-\lambda\mathbf{1}) = \tag{4.21}$$
$$\det(A_{11}-\lambda\mathbf{1})\bigg(\det(A-\lambda\mathbf{1}) + \det\begin{bmatrix} 0 & B_{12} \\ B_{21} & B_{22}-\lambda\mathbf{1}\end{bmatrix}\bigg). \tag{4.22}$$

Note that A and $\begin{bmatrix} 0 & B_{12} \\ B_{21} & B_{22}-\lambda\mathbf{1}\end{bmatrix}$ are both in $\in M_{\frac{N}{2}+1}(\mathbb{R})$. It is easy to see that the determinant of the latter matrix is given by

$$-\frac{B^2}{2}(1/2+1/N)\det(\tilde{A}-\lambda\mathbf{1}). \tag{4.23}$$

Here, $\tilde{A}\in M_{\frac{N}{2}-1}(\mathbb{R})$ is the matrix A_{11}, but with the last row and column deleted.
We write

$$\begin{aligned} p_{\frac{N}{2}+1}(\lambda) &= \det(A-\lambda\mathbf{1}), \\ p_{\frac{N}{2}}(\lambda) &= \det(A_{11}-\lambda\mathbf{1}), \\ p_{\frac{N}{2}-1}(\lambda) &= \det(\tilde{A}-\lambda\mathbf{1}), \end{aligned} \tag{4.24}$$

the characteristic polynomials of the matrices A, A_{11} and $\tilde{A}$ respectively. Finally, we put

$$b_{N/2} = -B\sqrt{1/2(1/2+1/N)}. \tag{4.25}$$

Then, in this notation, we have showed that

$$\det(J_{N+1}/N-\lambda\mathbf{1}) = p_{\frac{N}{2}}(\lambda)\bigg(p_{\frac{N}{2}+1}(\lambda) - b_{N/2}^2 p_{\frac{N}{2}-1}(\lambda)\bigg). \tag{4.26}$$

□

The eigenvalues are obtained by setting the above equation equal to zero. We know by Theorem 4.1 that all eigenvalues are distinct for each N, so that the characteristic polynomials factors completely. However, it is still extremely difficult to find the exact eigenvalues, since we do not know the functions $p_{\frac{N}{2}}$ exactly. Moreover, it is a priori not clear how the zeros of $p_{\frac{N}{2}}$ are related to the zeros of $p_{\frac{N}{2}\pm 1}$. Fortunately, from numerical simulations, we do have a relation between some of the zeros of the different characteristic polynomials. This is stated in a conjecture below.

Conjecture 4.1. *The smallest two zeros $\lambda^i_{\frac{N}{2}}$ and $\lambda^i_{\frac{N}{2}\pm 1}$ of the characteristic polynomials $p_{\frac{N}{2}}$ and $p_{\frac{N}{2}\pm 1}$ respectively, defined above, satisfy the inequality*

$$|\lambda^i_{\frac{N}{2}} - \lambda^i_{\frac{N}{2}\pm 1}| \leqslant \frac{C}{N^2}, \quad (i = 0, 1), \tag{4.27}$$

for sufficiently large N, i.e. there is a natural number N_0 and a real number $C > 0$ such that for any $K > N_0$, we have

$$|\lambda^i_{\frac{K}{2}} - \lambda^i_{\frac{K}{2}\pm 1}| \leqslant \frac{C}{K^2}, \quad (i = 0, 1). \tag{4.28}$$

Assuming this statement is true, we can use this result to say something more about (4.9). Setting $\det(J_{N+1}/N - \lambda \mathbf{1}) = 0$, it follows that

$$p_{\frac{N}{2}}(\lambda)p_{\frac{N}{2}+1}(\lambda) = b^2_{N/2}p_{\frac{N}{2}}(\lambda)p_{\frac{N}{2}-1}(\lambda). \tag{4.29}$$

By the previous theorem, we have $\lambda^i_{\frac{N}{2}} \approx \lambda^i_{\frac{N}{2}\pm 1}$, for N sufficiently large en i small. Since polynomials are determined by its zeros, one might expect that for these values of N the polynomials $p_{\frac{N}{2}}$ and $p_{\frac{N}{2}\pm 1}$ are approximately equal on an interval of the domain where these zeros are located.
As $b^2_{N/2} \neq 0$ for any N, this will indeed confirm that the eigenvalues become approximately doubly degenerate.
Keep still in mind that this approximation of degeneracy will never become an equality, since N needs to be finite in order to speak about a proper quantum system, and hence about eigenvalues, in the first place. As we have mentioned before, we will explain this in detail in §4.6. Moreover, it is not clear what the limit of such a polynomial will be.

4.4 Link with orthogonal polynomials

In this section we will use orthogonal polynomials to deduce some properties of our tridiagonal matrix. We are given the $N + 1$-dimensional Curie-Weiss Hamiltonian, written with respect to the canonical base for the subspace $\mathrm{Sym}^N(\mathbb{C}^2)$ of $\bigotimes_{n=1}^N \mathbb{C}^2 \cong \mathbb{C}^{2^N}$. The corresponding matrix representation was denoted by J_{N+1}. We again put $B = 1/2$ and $J = 1$.

If v is an eigenvector of J_{N+1}, then we can write $J_{N+1}v = \lambda v$ with $v = \sum_{i=0}^N \mu_i e_i \neq 0$, where $\{e_i\}$ is the standard basis for $\mathbb{C}^{N+1}$. As the matrix is real and symmetric, the coefficients μ_i are real. We denote the diagonal terms by b_i and the off-diagonal terms by a_i. In this notation we have

$$J_{N+1}e_i = a_{i-1}e_{i-1} + b_i e_i + a_{i+1}e_{i+1}, \tag{4.30}$$

and

$$J_{N+1}\sum_{i=0}^{N}\mu_i e_i = \sum_{i=0}^{N}\mu_i J_{N+1}e_i = \tag{4.31}$$

$$\sum_{i=0}^{N}\mu_i(a_{i-1}e_{i-1} + b_i e_i + a_{i+1}e_{i+1}) = \tag{4.32}$$

$$\sum_{i=0}^{N}(\mu_{i+1}a_i + b_i\mu_i + a_i\mu_{i-1})e_i. \tag{4.33}$$

It follows that

$$\lambda\mu_i = a_i\mu_{i+1} + b_i\mu_i + a_i\mu_{i-1} \quad i = 0, ..., N, \tag{4.34}$$

with $\mu_0 = 1$ and $\mu_{-1} = 0$. This is a three-term recurrence relation associated to the symmetric tridiagonal matrix J_{N+1}. Since the diagonal entries are all real and the off-diagonal terms are all strictly negative for each N, the corresponding infinite matrix J_∞ is a Jacobi matrix.[2] However, we will always focus on the semiclassical regime, i.e., for large, but finite N. One can try to solve this recurrence relation using discrete orthogonal polynomials $\{P_i\}_{i=0}^N$. Then the above equation reads

$$\lambda P_i(\lambda) = a_i P_{i+1}(\lambda) + b_i P_i(\lambda) + a_i P_{i-1}(\lambda) \quad i = 0, ..., N, \tag{4.35}$$

with $P_0(\lambda) = 1$, and $P_{-1}(\lambda) = 0$ and with λ in the spectrum of J_N. If we normalize this relation, we find that the above equation is equivalent to

$$\lambda P_i(\lambda) = P_{i+1}(\lambda) + b_i P_i(\lambda) + a_{i-1}^2 P_{i-1}(\lambda). \tag{4.36}$$

Plugging in the expressions for b_i and a_i gives

$$\lambda P_i(\lambda) = P_{i+1}(\lambda) - \frac{1}{2N}(2i - N)^2 P_i(\lambda) - \frac{1}{4}((N + 1 - i)i)P_{i-1}(\lambda). \tag{4.37}$$

Note that these coefficients are unbounded in N. The coefficients of the above normalized recurrence relation look a bit like the ones from Krawtchouk as explained in [20] for $p = 1/2$, since his normalized recurrence relation is given by

$$\lambda P_i(\lambda) = P_{i+1}(\lambda) - [p(N - i) + i(1 - p)]P_i(\lambda) - ip(1 - p)(N + 1 - i)P_{i-1}(\lambda). \tag{4.38}$$

Unfortunately, for $p = 1/2$, only the term in front of $P_{i-1}(\lambda)$ will match the corresponding one in our recurrence relation. The Askey scheme [20] has been checked and there is no known classical orthogonal polynomial that solves our recurrence relation. So the approach through orthogonal polynomials seems a dead end, but it was worth a try.

In the next paragraph, we are going to link the operator J_{N+1}/N to a Schrödinger operator. Thus, considering (4.37) for J_{N+1}/N, gives:

$$\lambda P_i(\lambda) = P_{i+1}(\lambda) - \frac{1}{2}(\frac{2i}{N} - 1)^2 P_i(\lambda) - \frac{1}{4}((1 - \frac{i}{N} + \frac{1}{N})\frac{i}{N})P_{i-1}(\lambda). \tag{4.39}$$

This time, the coefficients are bounded, but there it still no classical polynomial from the Askey scheme that solves this recurrence relation (4.39).

[2] A Jacobi matrix A is an infinite symmetric tridiagonal matrix with real diagonal coefficients, and non-zero off-diagonal coefficients that are all positive or all negative. The domain of the Jacobi matrix is defined as $D(A) = \{x \in \ell^2 |\ Ax \in \ell^2\}$.

For every finite N, each eigenvector of J_{N+1} is an element of $\mathbb{R}^{N+1}$ and therefore one can expand it in an orthonormal basis, say the standard one. If one can show that there exists polynomials $P_i(\lambda)$ such that the coefficients in this expansion are the same as the $P_i(\lambda)$ for $i = 0, ..., N$, which is then equivalent to the fact that these polynomials solve the recurrence relation, we are done.
We still don't know yet how to find these polynomials. The problem relies on the fact that in the normalized recurrence relation, there are two quadratic terms in i which makes that we cannot easily apply the Askey scheme.

4.5 Locally uniform discretization

In this section, we start giving the basic principles of discretization of a second order differential operator. We will do this on a uniform as well as on a non-uniform grid. Moreover, we make a link between symmetric tridiagonal matrices and a discretization of a Schrödinger operator. Secondly, we apply these result to the Curie-Weiss Hamiltoniann, written with respect to the canonical symmetric basis for the subspace $\mathrm{Sym}^N(\mathbb{C}^2)$ of $\otimes_{n=1}^N \mathbb{C}^2 \cong \mathbb{C}^{2^N}$. For reasons regarding SSB, we still fix $B = 1/2$ and $J = 1$ and keep these parameters fixed, unless specified otherwise. As before, we denote this matrix by J_{N+1}

Discretization is the process of approximating the derivatives in (partial) differential equations by linear combinations of function values f in so-called *grid points.* The idea is to discretize the domain, with N of such grid points, known as a *grid*. We give an example in one dimension.

$$\Omega = [0, X], \qquad f_i \approx f(x_i), \qquad (i = 0, .., N), \tag{4.40}$$

with grid points $x_i = i\Delta$ and grid size $\Delta = X/N$. The symbol Δ is called the *grid spacing*. Note this the grid spacing is chosen to be constant or uniform in this specific example. For the first order derivatives (see also Appendix B), we have

$$\begin{aligned}\frac{\partial f}{\partial x}(\bar{x}) &= \lim_{\Delta x \to 0} \frac{f(\bar{x} + \Delta x) - f(\bar{x})}{\Delta x} \\ &= \lim_{\Delta x \to 0} \frac{f(\bar{x}) - f(\bar{x} - \Delta x)}{\Delta x} \\ &= \lim_{\Delta x \to 0} \frac{f(\bar{x} + \Delta x) - f(\bar{x} - \Delta x)}{2\Delta x}.\end{aligned} \tag{4.41}$$

These derivatives are approximated with *finite differences*. There are basically three types of such approximations:

$$\begin{aligned}\left(\frac{\partial f}{\partial x}\right)_i &\approx \frac{f_{i+1} - f_i}{\Delta x} \quad \text{(forward difference)} \\ \left(\frac{\partial f}{\partial x}\right)_i &\approx \frac{f_i - f_{i-1}}{\Delta x} \quad \text{(backward difference)} \\ \left(\frac{\partial f}{\partial x}\right)_i &\approx \frac{f_{i+1} - f_{i-1}}{2\Delta x} \quad \text{(central difference).}\end{aligned} \tag{4.42}$$

It can be shown (Appendix B) that the central difference approximations are more accurate. Therefore, we will focus on the central difference approximation method and apply this to the second order differential operator d^2/dx^2. In the example above, the grid spacing was chosen to be uniform. Consider this example again, now on the domain $\Omega = [0, 1]$ with uniform grid spacing

$\Delta = 1/N$. It can be shown (using (B.12)), that the second order derivative operator is approximately given by

$$f_i'' \approx \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta^2} \quad (i = 1, ..., N), \tag{4.43}$$

where we have thrown away the error term term $O(h^2)$ in (B.12). It follows that we can write the second derivative operator in matrix form

$$\frac{1}{\Delta^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix} \tag{4.44}$$

This matrix is the standard discretization of the second order derivative on a uniform grid consisting of N points of length $\Delta \cdot N$, with uniform grid spacing Δ. In this specific case, we have $\Delta = 1/N$. We denote this matrix also by $\frac{1}{\Delta^2}[\cdots 1 \ -2 \ 1 \cdots]_N$.

Suppose now that we are given a symmetric tridiagonal matrix A of dimension N with constant off- and diagonal elements,

$$A = \begin{pmatrix} b & a & & & \\ a & b & a & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & a & b & a \\ & & & a & b \end{pmatrix} \tag{4.45}$$

We are going to extract a kinetic and a potential energy from this matrix. We write

$$A = a[\cdots 1 \ \frac{b}{a} \ 1 \cdots]_N = a[\cdots 1 \ -2 \ 1 \cdots]_N + \mathrm{diag}(b + 2a), \tag{4.46}$$

where the latter matrix is a diagonal matrix with the element $b+2a$ on the diagonal. It follows that

$$A = T + V, \tag{4.47}$$

for $T = a[\cdots 1 \ -2 \ 1 \cdots]_N$, and $V = \mathrm{diag}(b + 2a)$. In view of the above, the matrix T corresponds to a second order differential operator. This matrix plays the role of (4.44), but with uniform grid spacing $1/\sqrt{a}$ on the grid of length $N/\sqrt{a}$. Since the matrix V is a diagonal matrix, it can be seen as a multiplication operator. Therefore, given such a symmetric tridiagonal matix A, we can derive an operator that is the sum of a discretization of a second order differential operator and a multiplication operator. The latter operator is identified with the potential energy of the system. Hence, we can identify A with a discretization of a Schrödinger operator.[3]

The next step is to understand what happens in the case where we are given a symmetric tridiagonal matrix with non-constant off- and on-diagonal elements. This is important as we will see, since the Curie-Weiss Hamiltonian, written with respect to the canonical symmetric base for the subspace $\mathrm{Sym}^N(\mathbb{C}^2)$ of $\mathbb{C}^{2^N} \simeq \bigotimes_{n=1}^N \mathbb{C}^2$, is precisely an example of such matrix. The question we ask ourselves is if we can link such a matrix to a discretization of a Schrödinger operator as

[3]Strictly speaking we have to put a minus sign in front of T, as the kinetic energy is defined as $-\frac{d^2}{dx^2}$.

well.

Let us first review the second order differential operator $\frac{d^2}{dx^2}$. In most central finite difference applications *non-uniform grids* are employed, allowing the grid to be more refined in regions where strong gradients are expected. In that case the grid points x_i $(i = 1, ..., N)$ are not uniformly distributed over the domain. We define:

$$h_{j+\frac{1}{2}} = x_{j+1} - x_j \quad (i = 1, ..., N). \tag{4.48}$$

The length of the domain of discretization is then given by

$$\sum_{j=1}^{N} h_{j+\frac{1}{2}}. \tag{4.49}$$

Using a central difference approximation, it can be shown (see Appendix B, formula (B.16)) that the second order derivative is given by the expression

$$f_j'' = \frac{2f_{j-1}}{h_{j-\frac{1}{2}}(h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}})} - \frac{2f_j}{h_{j-\frac{1}{2}}h_{j+\frac{1}{2}}} + \frac{2f_{j+1}}{h_{j+\frac{1}{2}}(h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}})}. \tag{4.50}$$

Again, we have thrown away the error term $O(h^2)$, and we assumed that we may neglect the relative small term $h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}}$ in (B.16). Like for (4.44), we can also derive a matrix for the second order derivative. This time the matrix entries are non-constant and they are given by (B.17), (B.19) and (B.18).

Finally, suppose we are given a symmetric tridiagonal matrix B with non-constant off- and on-diagonal elements. As for the uniform case, the question we asked ourselves was whether we can link this matrix to a discretization of a Schrödinger operator. Note that we cannot easily apply the same procedure as in the uniform case since, the matrix entries are not constant. Therefore, we identify the matrix B with (4.50). It follows that

$$B_{j,j+1} = \frac{2}{h_{j+\frac{1}{2}}(h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}})}, \tag{4.51}$$

$$B_{j,j} = \frac{-2}{h_{j-\frac{1}{2}}h_{j+\frac{1}{2}}}, \tag{4.52}$$

$$B_{j,j-1} = \frac{2}{h_{j-\frac{1}{2}}(h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}})}. \tag{4.53}$$

We can compute the non-uniform grid spacing $h_{j+\frac{1}{2}}$ as follows. We put

$$\rho_j = \frac{B_{j,j+1}}{B_{j,j-1}} = \frac{h_{j-\frac{1}{2}}}{h_{j+\frac{1}{2}}}. \tag{4.54}$$

We derive from this combined with the above three equations that

$$h_{j+\frac{1}{2}}^2 = \frac{2}{B_{j,j+1}(1 + \rho_j)}. \tag{4.55}$$

From (4.53), we also find

$$h_{j-1/2}^2 = \frac{2}{B_{j,j-1}(1/\rho_j + 1)}. \tag{4.56}$$

From $h_{(j-1)+1/2} = h_{j-1/2}$, it now follows that

$$\rho_{j-1} = \frac{1}{\rho_j}, \quad \text{or equivalently,} \tag{4.57}$$

$$B_{j+1,j} = B_{j-1,j-2}, \text{ and } B_{j,j-1} = B_{j-2,j-3}, \tag{4.58}$$

where we used the fact that that the matrix is symmetric. This means that the off-diagonal matrix entries of B must have the form $c, d, c, d, c, d, ...,$. If this is the case, then indeed we can identify B with a discretization of a second order differential operator. This is clearly true for (4.45), since the off-diagonal entries are all equal. Moreover, the potential energy is then obtained by subtracting (4.52) from the diagonal of B. The result is that such a tridiagonal matrix with this symmetry of the off-diagonal elements can also be written as sum of a kinetic and a potential energy operator and hence corresponds to a discrete analog of a one-dimensional Schrödinger operator in a potential well.

This closes the first part of this section. In the next part, we apply these result to our tridiagonal matrix J_{N+1}. Our goal is to explain that J_{N+1} *locally approximates* a discretization matrix of the form (4.45) (for N large) corresponding to a Schrödinger operator that describes a particle in a symmetric double well potential. This means that there exists a sub-block of J_{N+1} that has the form approximately given by the sum of $\frac{1}{h^2}[\cdot\cdot\cdot 1 \;\; -2 \;\; 1 \cdot\cdot\cdot]$ (for some h to be determined) and a diagonal matrix playing the role of a potential. This implies that the matrix J_{N+1} applied to vectors that are nonzero on some subset W of the domain[4], and zero outside W, yields the same vectors as the discretization matrix applied to these vectors.[5] Indeed, the existence of such a sub-block explained above is equivalent to the existence of the subset W of the domain of discretization on which this discretization is approximately uniform (which meaning has been explained at the beginning of this section).[6] In §4.6 we will derive an explicit formula for this discretization matrix. Moreover, we will see that to a very good approximation even the spectral properties of both different matrices coincide and that this approximation gets better with increasing N. In §4.7, we finally explain how to link this matrix to a Schrödinger operator on $L^2([0,1])$. For the remaining part of this section we are going to show the extremely important fact that grid spacing is approximately constant on some subset of the domain of discretization. This observation is the basis of the link with the Schrödinger operator.

Thus consider the matrix J_{N+1}. This matrix is tridiagonal with non-constant off- and diagonal entries. In view of the above, we therefore apply the non-uniform discretization process in order to identify this matrix with a discretization of a second order derivative operator and a multiplication operator. At first sight, for any finite $N > 0$, the matirix J_{N+1} does not have off-diagonal elements of the form $c, d, c, d, c, d, ...,$, let alone $c, c, c, c, ...,$. However, we will argue (details given in §4.6 and §4.7) that the scaled matrix J_{N+1}/N locally approximates some discretization matrix à la (4.45) corresponding to a Schrödinger operator describing a particle in a symmetric double well potential, for large, but finite N. In order to show this, we see in this paragraph that in the limit $N \to \infty$ we have uniform discretization on some interval, even though the limit point at $N = \infty$ does not exists. Making N large enough, this discretization will be already almost uniform and thus we have an approximate kinetic energy with emergent Schrödinger operator.

[4]We identify the subset W of the domain of discretization (which is some subset of $\mathbb{R}$) with a subspace of the vector space $\mathbb{R}^N$, where N denotes the number of grid points.

[5]Strictly speaking this is not true since the discretization is *approximately* uniform, so that the off- and diagonal matrix entries are not constant. They are only constant in an approximation.

[6]We will stick to this notion of 'locally approximation' in the remaining part of this paragraph and chapter.

We write $T = J_{N+1}$. Then as before, consider the ratios:

$$\rho_j = \frac{h_{j-1/2}}{h_{j+1/2}} = \frac{T_{j+1}}{T_{j-1}} \quad (j = 1, ..., N), \tag{4.59}$$

with non-uniform grid spacing $h_{j\pm1/2}$. We divide the original tridiagonal matrix J_{N+1} by N for scaling. Thus, we consider J_{N+1}/N. If we then compute the distances $h_{j+1/2}$, we see that they are almost all of $O(1)$, except at the boundaries. Since we then have approximately N distances of each order 1, we will see later that the corresponding Schrödinger operator analog of the matrix J_{N+1}/N will be an operator on a domain of length of order N.

First, we compute the ratios ρ_j:

$$\rho_j = \frac{T_{j+1}}{T_{j-1}} = \frac{\sqrt{(N-j)(j+1)}}{\sqrt{(N-j+1)j}} = \sqrt{\frac{N-j}{N-j+1}}\sqrt{\frac{j+1}{j}} = \sqrt{\frac{1}{1+\frac{1}{N-j}}}\sqrt{1+\frac{1}{j}}. \tag{4.60}$$

Since

$$\sqrt{1+\frac{1}{j}} \approx 1 + \frac{1}{2j} = 1 + O(1/j) \quad \text{and} \tag{4.61}$$

$$\sqrt{\frac{1}{1+1/(N-j)}} \approx 1 - \frac{1}{2(N-j)} = 1 + O\bigg(\frac{1}{N-j}\bigg), \tag{4.62}$$

we see that the ratio satisfies

$$\rho_j \approx 1 + O(1/j) + O\bigg(\frac{1}{N-j}\bigg), \tag{4.63}$$

using the fact that that the big-O notation respects the product, that $O(\frac{1}{j}\frac{1}{N-j}) \leqslant O(1/j)$, and also $O(\frac{1}{j}\frac{1}{N-j}) \leqslant O(\frac{1}{N-j})$.

In the next paragraph, we will see from numerical simulations that to a good approximation the ground state eigenfunction is a double peaked Gaussian with maxima centered in the minima of some double well potential that we are going to determine. This potential occurs in a discrete Schrödinger operator analog of the matrix J_{N+1}/N for N large, i.e., in the semiclassical limit.
By these calculations, it follows that when we map the double well on the unit interval the two minima of the symmetric double well are given by

$$\frac{1}{2} \pm \frac{1}{4}\sqrt{3}. \tag{4.64}$$

These minima are of order 1, and when we consider the potential on the original domain of order N, the minima are (compared to N) of order

$$N\bigg(\frac{1}{2} \pm \frac{1}{4}\sqrt{3}\bigg) = O(N). \tag{4.65}$$

Furthermore, we showed by numerical simulations (Figure 4.1 below) that the width σ of each Gaussian-shaped[7] ground state of J_{N+1} located at one of minima of the potential is of order $\sqrt{N}$, and hence that each peak rapidly decays to zero, so that the ground state eigenfunction is approximately zero at both boundaries. In particular, the domain where the peak is non-zero is of order $\sqrt{N}$, as we clearly observe from the figure. This is an approximation, since we neglect the (relatively small) function values of the Gaussian that are more than $O(\sqrt{N})$ away from the central maximum. However, this approximation is reasonable, as the Gaussian decays to zero exponentially.

[7]We mean that if we plot the discrete points and draw a line through these points, then the corresponding graph has the shape of a Gaussian.

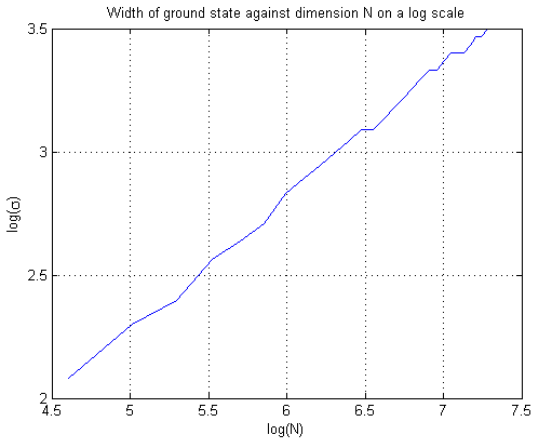

Figure 4.1: The width at half height of the ground state eigenvector of J_{N+1} ($B = 1/2$ and $J = 1$) against N, for $N = 100 : 50 : 1500$ on a log scale. The slope of the line is about 0.5, which means that the width σ goes like $\sqrt{N}$.

This observation (the plot above) is extremely important, as we will see now.

Let us first focus on the left-located Gaussian. For a point j in the domain of order N, clearly $j \in O(N)$. Therefore, for N large enough,

$$\rho_j \approx 1 + O(1/N), \tag{4.66}$$

since for these values of $j < N - j$ we have $O(\frac{1}{N-j}) \leqslant O(1/j)$. For the right-located peak, we have $N - j < j$, so that in this case $O(1/j) \leqslant O(\frac{1}{N-j})$, and we find

$$\rho_j \approx 1 + O\left(\frac{1}{N-j}\right). \tag{4.67}$$

We will now show that on an interval of length of order $\sqrt{N}$, we indeed have uniform discretization.

We start with the peak on the left. Since the error per step that we make equals ρ_j, it follows that the error on the interval of length of order σ, equals $\rho_j^\sigma \approx (1 + \frac{1}{N})^\sigma$ for $j < N - j$ and N large.

Denoting the off-diagonal element corresponding to the minimum x_{j_0} of the potential well by T_{j_0}, for the off-diagonal elements within a range of order σ, we derive the next estimate:

$$|T_{j_0} - T_{j_0+\sigma}| \approx |T_{j_0} - O\left((1 + \frac{1}{N})^\sigma\right)T_{j_0}| = T_{j_0}|1 - O\left((1 + \frac{1}{N})^\sigma\right)| \leqslant C\frac{\sigma}{N}, \tag{4.68}$$

where we used $(1 + 1/N)^\sigma \leqslant 1 + C\frac{\sigma}{N}$ and the fact that T_{j_0} is of order 1. Here, $C > 1$ is a constant independent of N.

Since the left peak of the Gaussian eigenfunction is approximatley non-zero within an interval of length of order $\sqrt{N}$, we apply the above estimate to $\sigma \approx \sqrt{N}$. We see immediately that $|T_{j_0} - T_{j_0+\sigma}|$ goes to zero. Therefore, on an interval of length of order $\sqrt{N}$ centered around the left minimum x_{j_0} of the potential, the off-diagonal elements become the same in the limit $N \to \infty$. This means that the grid spacing becomes constant and hence that we have locally uniform discretization of the domain. By symmetry, the same is true for the peak located on the right of the well. We conclude

that the tridiagonal matrix locally behaves like a kinetic energy (and therefore like a discretized Schrödinger operator). This is an approximation, because we may only consider finite N. All this will be explained in more detail in the next two paragraphs.
Furthermore, note that this result is independent of the location of the interval of order $\sqrt{N}$. However, since we observe numerically that the Gaussian-shaped ground state located in the domain of order N attains its maxima at $N(\frac{1}{2} \pm \frac{1}{4}\sqrt{3})$ and exponentially decays to zero, the only interval that might play a role is the one centered around these maxima. We come back to this point in the next paragraph.

4.6 Link with a discrete Schrödinger operator

As we have already mentioned in the previous paragraph, our aim is to show that the matrix J_{N+1}/N locally approximates a discretization matrix corresponding to a Schrödinger operator describing a particle in a symmetric double well. We started with the symmetrix tridiagonal matrix J_{N+1}/N with non-constant entries. In order to link this matrix to a second derivative and a multiplication operator, we needed to apply the non-uniform discretization procedure. The off-diagonal matrix entries of J_{N+1}/N do not have the form $c, d, c, d, c, d, ...$, for any finite N. Therefore, we could not immediately identify this matrix with a second order derivative operator. However, we have seen in the limit $N \to \infty$, that we have uniform discretization on some interval of the total domain of discretization. Consequently, for sufficiently large, but finite N, this discretization becomes approximately uniform. From this fact, we will extract a matrix of the form (4.45) corresponding to a Schrödinger operator on $L^2([0,1])$. We now state the main results of this paragraph and §4.7. For this, we consider the matrix $\tilde{H}_N$, defined as

$$\tilde{H}_N = \tilde{T}_N + \tilde{V}_N, \tag{4.69}$$

where

$$\tilde{T}_N = -\frac{1}{8}[\cdots 1 \ -2 \ 1 \cdots]_N \tag{4.70}$$

and $\tilde{V}_N$ a diagonal matrix given by

$$\tilde{V}_N = -\frac{1}{2}(\frac{2j}{N} - 1)^2 - B\left(\sqrt{(1 - \frac{j}{N})(\frac{j}{N} + \frac{1}{N})} + \sqrt{(1 - \frac{j}{N} + \frac{1}{N})\frac{j}{N}})\right), \quad (j = 1, ..., N). \tag{4.71}$$

We show that the matrix J_{N+1}/N locally approximates $\tilde{H}_{N+1}$ for N large, but finite. Recall that this means that there exists some subset of the total domain of discretization on which the discretization is approximately uniform (with grid spacing approximately given by $\sqrt{8}$), and gets better with increasing N. This in turn means that the matrix J_{N+1}/N contains a sub-block of the form approximately given by the sum of $-\frac{1}{8}[\cdots 1 \ -2 \ 1 \cdots]_{N+1}$ and a diagonal matrix, given by (4.71). We see in this section that to a very good approximation even the spectral properties of both matrices coincide and get better with increasing N. In §4.7, we show that the matrix $\tilde{H}_N$ is a discretization of a Schrödinger operator on $L^2([0,1])$, denoted by $\tilde{h}_2$ and defined as

$$\tilde{h}_2 = -C_N \frac{1}{8}\frac{d^2}{dy^2} + m_{\tilde{V}}, \tag{4.72}$$

with $C_N = N^{-2}$. The potential $\tilde{V}$ (for $B = 1/2$ and $J = 1$) is then given by the continuous function

$$\tilde{V}(y) \approx -\frac{1}{2}(2y - 1)^2 - \sqrt{(1 - y)y}, \quad y \in [0, 1]. \tag{4.73}$$

For $\hbar = \frac{1}{N}$, we recognize the well-known Schrödinger operator (2.46). It is now clear why N needs to be finite: the case $N = \infty$ (or $\hbar = 0$) implies that the Schrödinger operator is no longer defined.

The next step is to show that the matrix $\tilde{H}_{N+1}$ defined by (4.69) can be indeed locally approximated by J_{N+1}/N. As we have seen in the previous paragraph, for N large enough, we locally have an approximate uniform discretization of the domain of discretization, using the fact that some of the off-diagonal elements are approximately constant. Similar as for (4.45) explained in §4.5, this implies that we can identify a sub-block of this matrix with a second order derivative and hence with a kinetic energy T and a potential V. The latter operator is obtained by subtracting the kinetic energy contribution to the diagonal from the diagonal of the original matrix J_{N+1}/N. Let us first focus on the kinetic energy. As explained in §4.5, we want to identify this sub-block to a kinetic energy operator of the form:

$$T = -\frac{1}{h^2}\,[\cdots 1 \;\; -2 \; 1 \cdots]. \tag{4.74}$$

This matrix is the second-order derivative on a grid of length $h \cdot \dim(\text{sub-block})$, where the dimension of this sub-block is approximately equal to $\sqrt{N}$, as explained in the last part of §4.5. The constant h denotes the uniform grid spacing.[8] This value can be determined using Appendix B or §4.5. The value of h is fixed by (B.22), i.e.,

$$h_{j+1/2} = \sqrt{-\frac{2}{T_{j,j+1}(1+\rho_j)}}. \tag{4.75}$$

As we know, for large N, the values $h_{j+\frac{1}{2}}$ are approximately constant on some specific subset of the domain. This subset was located around the maxima of both Gaussian-shaped ground state peaks. If we then denote the grid spacing at the central maximum of both Gaussians by $h_{j_0+\frac{1}{2}}$, we find numerically that $h^2_{j_0+\frac{1}{2}} \approx 8$, for $N = 5000$. This approximation gets better for increasing N. Moreover, we observe also from numerical calculations that the approximation of the number 8 by $h^2_{j+1/2}$ becomes better for those values of $h_{j+1/2}$ that belong to the entire subset of $O(\sqrt{N})$, when N gets larger. This verifies that the subdomain centered around x_{j_0} is uniformly discretized with grid spacing $h = \sqrt{8}$. We have shown that the matrix J_{N+1}/N contains a sub-block[9] for which the kinetic energy is approximately given by (4.74), for $h = \sqrt{8}$. Since we have seen that locally around the maxima of both Gaussians the kinetic energy contribution to the diagonal approximately equals $2/h^2 \approx 1/4$, it follows that the potential V is locally approximately given by

$$V \approx \operatorname{diag}(J_{N+1}/N) - 1/4. \tag{4.76}$$

Hence, the matrix J_{N+1}/N contains two sub-blocks that can be approximately written as sum of a kinetic energy T and a potential energy V. We will see that the potential V approximately equals the matrix $\tilde{V}_N$ (defined by (4.71)) locally around both maxima of the Gaussians. By definition of $\tilde{H}_N$, it then follows that the matrix J_{N+1}/N applied to vectors living on this subset of the domain of order $\sqrt{N}$ on which the discretization is approximately uniform, and are zero outside this set, approximately yields the same vectors as the matrix $\tilde{H}_{N+1}$ applied to these vectors. This indeed shows that the matrix $\tilde{H}_{N+1}$ can be locally approximated by J_{N+1}/N.

The next step in the process of the analysis regarding the matrix $\tilde{H}_N$ is to explain how the potential $\tilde{V}_N$ given by (4.71) is obtained.

[8] Note that this result is in accordance with (4.47) for $a = 1/h^2$, since the corresponding grid spacing is $1/\sqrt{a} = h$.

[9] By symmetry of the ground state, there are two subsets of order $\sqrt{N}$ on which the discretization is uniform. As a result, the matrix J_{N+1}/N contains two of such sub-blocks.

In order to find this matrix $\tilde{V}_N$, we start again with J_{N+1}/N. We apply the same procedure as before, namely, we first compute the contribution of the 'kinetic energy' $\tilde{K}_N$ to the diagonal of J_{N+1} on the *entire* domain of discretization, using the formula

$$\tilde{K}_N(j,j) = -\frac{2}{\rho_j h_{j+1/2}^2} \quad (j = 1, ..., N+1). \tag{4.77}$$

We use quotation marks to indicate that $\tilde{K}_N$ is not a kinetic energy, because the discretization is not uniform globally.[10] We just use this as a trick to compute $\tilde{V}_N$ for the matrix $\tilde{H}_N$. As before, we compute $\tilde{V}_N$ by

$$\tilde{V}_N = \mathrm{diag}(J_{N+1}/N) - \tilde{K}_N(j,j), \quad (j = 1, ..., N+1). \tag{4.78}$$

We are going to simplify (4.78). We start with J_{N+1}. Write $\tilde{K}_N(k,j) \equiv \tilde{K}_{k,j}$, $\tilde{V}_N(k,j) \equiv \tilde{V}_{k,j}$ and $J_{N+1}(k,j) \equiv J_{k,j}$. Elaborating formula (4.77) for $\tilde{K}_N$ gives

$$\tilde{K}_{j,j} = -(J_{j,j-1} + J_{j,j+1}), \tag{4.79}$$

where $J_{j,j\pm1}$ are the off-diagonal entries of the tridiagonal matrix J_{N+1}. Plugging in the expressions for $J_{j,j\pm1}$, shows that the above equation is equal to

$$\tilde{K}_{j,j} = B(\sqrt{(N-j)(j+N)} + \sqrt{(N-j+1)j}). \tag{4.80}$$

It follows that (4.78) reads

$$\tilde{V}_{j,j} = J_{j,j} - (-(J_{j,j-1} + J_{j,j+1})). \tag{4.81}$$

One should mention that the above equation (4.81) approximately equals formula (4.76) since $\tilde{T}_{j,j} \approx \frac{1}{4}$, locally around the maxima of the Gaussians for N large enough. This is almost exact when N is large enough, since on this subset we may indeed speak about uniform discretization and thus a kinetic energy.

Plugging in he expressions for $J_{j,j}$ and $T_{j,j\pm1}$ gives

$$\tilde{V}_{j,j} = -\frac{1}{2N}(2j-N)^2 - B(\sqrt{(N-j)(j+1)} + \sqrt{(N-j+1)j}). \tag{4.82}$$

Using the identity $j = \frac{jN}{N}$, the above expression (4.82) for the potential equals

$$\tilde{V}_{j,j} = N\bigg(-\frac{1}{2}(\frac{2j}{N} - 1)^2 - B(\sqrt{(1-\frac{j}{N})(\frac{j}{N}+\frac{1}{N})} + \sqrt{(1-\frac{j}{N}+\frac{1}{N})\frac{j}{N}})\bigg). \tag{4.83}$$

Then for J_{N+1}/N, we see that the factor N in front of the above equations disappears. With abuse of notation, we put $\tilde{V}_N \equiv \tilde{V}/N$. Note that $\tilde{V}_N$ is indeed given by (4.71). Then using (4.70) for the kinetic energy, we define the $(N \times N)$-matrix $\tilde{H}_N$ by

$$\tilde{H}_N = \tilde{T}_N + \tilde{V}_N. \tag{4.84}$$

This shows how the potential $\tilde{V}_N$ and therefore the matrix $\tilde{H}_N$ is constructed. As we will see in §4.7, this is in fact a discretization of the Schrödinger operator (4.72).

We have to be careful with the domain of the matrix J_{N+1}/N. The length of the domain

[10] This follows from the fact that ρ_j is not approximately equal to one for *all* $i = 1, ..., N+1$.

is given by the sum of all distances $h_{j+1/2}$. Here, j runs from 0 to N. We computed this length and this approximately gives $2.4N$, for N large enough. Therefore, each point x_j in the domain corresponds to the sum $\sum_{k=1}^{j} h_{k+1/2}$. In particular, $\sum_{k=1}^{n} h_{k+1/2} \approx 2.4N$. However, as we have just seen, the operator $\tilde{T}_N$ and hence $\tilde{H}_N$ are defined on a domain of approximate length of $\sqrt{8}N$, which is fortunately the same order as $2.4N$.

Remark. Consider the Schrödinger operator with a symmetric double well potential, given by (2.46). Recall from §3.2 that for a sufficiently high and broad potential well, the ground state of such a Schrödinger operator is approximately given by two Gaussians, each of them located in one of the wells of the potential. This fact will be useful for the next observations.

We will now see that the Gaussian-shaped ground state of J_{N+1}/N, indeed localizes in both minima of the potential well $\tilde{V}_N$. Therefore, we have made a plot of the scaled potential $\tilde{V}_N$ from equation (4.83) on the domain of length $2.4N$, for $B = 1/2$ and $J = 1$. See Figure 4.2 below. We immediately recognize the shape of a symmetric double well potential. The points in its domain are given by $x_j = \sum_{k=1}^{j} h_{k+1/2}$ for $j = 0, ..., N$. Then we diagonalized the matrix J_{N+1}/N and computed the ground state eigenvector. We plot this together with the potential in Figure 4.2. One should mention that there is only one Gaussian peak visible, not two. As we have seen in §3.2, this was due to the (in)accuracy of the computer i.e., the first two eigenvalues are already degenerate. Therefore, the system is completely decoupled and thus the computer randomly picks one of the two Gaussians as ground state, even though we know from the Perron-Frobenius Theorem (Chapter 5) that the ground state is always unique for any finite N. We also observe that the maxima of the Gaussian ground state peaks are precisely centered in the minima of these two wells (as should be the case).

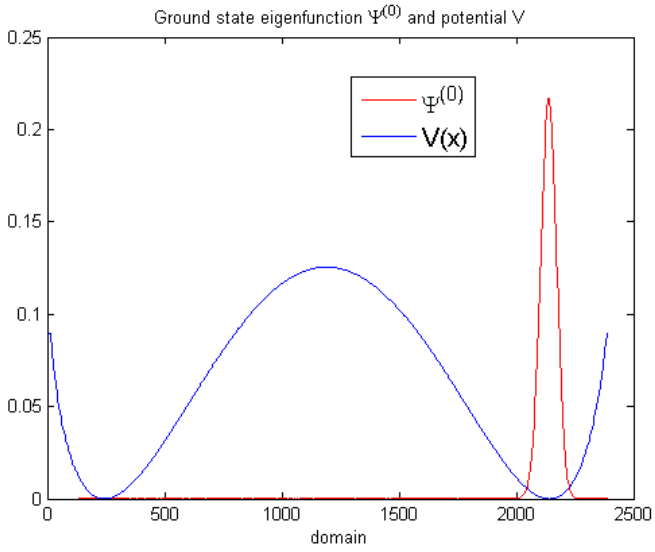

Figure 4.2: The scaled potential $\tilde{V}_N$ and the ground state eigenfunction corresponding to J_{N+1}/N for $N = 1000$. The potential is shifted so that its minimum is zero. The length of domain is approximately equal to $2.4N$ as explained above. The parameters $B = 1/2$ and $J = 1$ are still fixed.

From this figure, it is immediately clear that the ground state is localized in (one of the) minima of the double well.

One might suggests that there would be some critical value of N for which the eigenvalues are not yet degenerate for the computer. We have seen that this value of N is about $N = 80$. We

made a similar plot for the ground state for $N = 60$, like Figure 3.1 in §3.2. We recognize the well-known doubly peaked Gaussian shape, but now it is localized in both minima of the potential well. This is displayed in Figure 4.3. These figures show that there is a convincing relation between the matrix J_{N+1}/N and a Schrödinger operator describing a particle in a double well.

The double well shaped potential is a result of the choice $B = 1/2$. The value of the magnetic field needs to be within $[0, 1)$ in order to get spontaneous symmetry breaking of the ground state in the classical limit $N \to \infty$. For $B \geqslant 1$ the Curie-Weiss model will not display SSB, not even in the classical limit. In §6.3, two different classical limits will be discussed. One of them corresponds to the double well potential. Without going into details now, it is a fact that the classical limit of a Schrödinger operator with a symmetric double well potential corresponds to a doubly degenerate ground state that breaks the $\mathbb{Z}_2$-symmetry. For a single well potential, the classical limit is non-degenerate and does not break the symmetry. As we will see soon, the matrix J_{N+1}/N is a discretization of such a Schrödinger operator on $L^2([0, 1])$. However, the parameter B determines the shape of the well. For $B \geqslant 1$, the well will be a single potential. This is clear from Figure 4.4. In view of the corresponding Schrödinger operator, the ground state in the classical limit will not break the symmetry for a single potential well, and is therefore also compatible with the Curie-Weiss model for $B \geqslant 1$. This result is also in accordance with the Quantum Iisng model [22, Thm. 10.11].

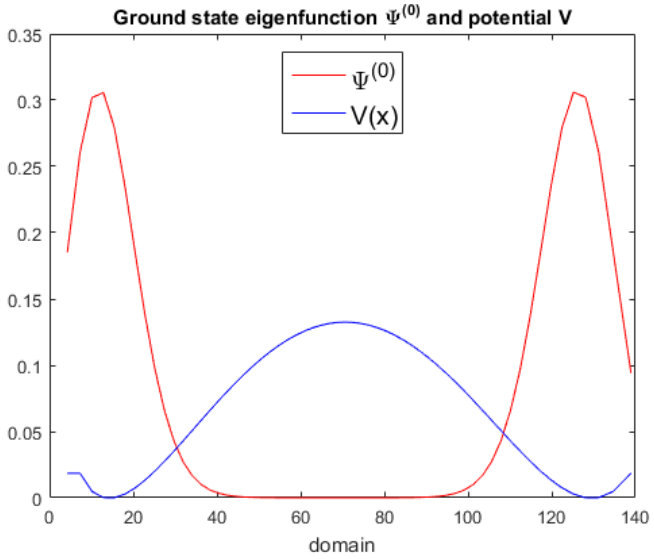

Figure 4.3: The scaled and shifted potential $\tilde{V}_N$ from the previous figure, and the ground state eigenfunction corresponding to J_{N+1}/N for $N = 60$. Also here, the length of domain is approximately $2.4N$. The ground state (discrete) eigenvector is normalized to 1.

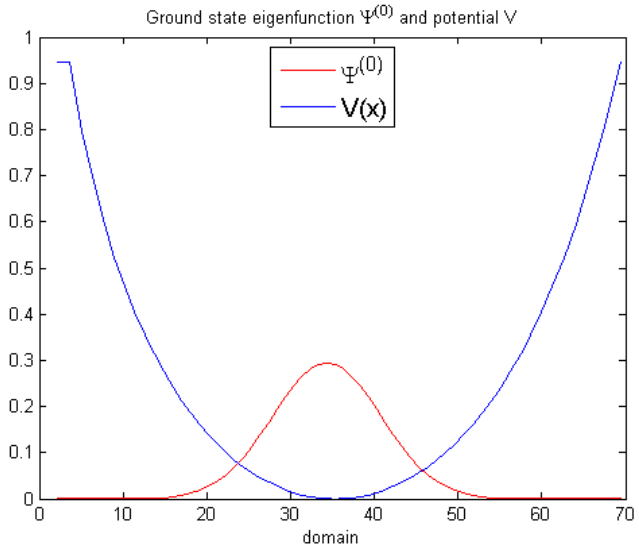

Figure 4.4: The scaled and shifted potential $\tilde{V}_N$ for $B = 2$ and $J = 1$, and the ground state eigenfunction corresponding to J_{N+1}/N for $N = 60$. The single well is clearly visible. Also now, the ground state eigenvector is normalized to 1.

We now turn back to the regime $0 \leqslant B < 1$. One can compute the spectral properties of the matrix J_{N+1}/N and compare them with those of the operator $\tilde{H}_N$. This will be the next step. We will see that to a very good approximation the spectral properties of both matrices coincide and get better with increasing N. We have programmed the matrix $\tilde{H}_N$ in MATLAB. The matrix has been diagonalized. The spectral properties have been compared to those of J_{N+1}/N. In the table below, the first 10 eigenvalues denoted by λ_n are displayed for the operator $\tilde{H}_N$. The same is done for the matrix J_{N+1}/N. These eigenvalues are denoted by ϵ_n. The number $N = 1000$ is fixed.

Eigenvalues		
n	λ_n	ϵ_n
0	-0.6251	-0.6251
1	-0.6251	-0.6251
2	-0.6234	-0.6234
3	-0.6234	-0.6234
4	-0.6217	-0.6217
5	-0.6217	-0.6217
6	-0.6200	-0.6200
7	-0.6200	-0.6200
8	-0.6183	-0.6183
9	-0.6183	-0.6183

We see that these ten eigenvalues are exactly the same for both systems up to four decimals. Our simulations showed that the eigenvalues differ from the sixth decimal for $n = 0, 1, 2, 3, 4$ and from the fifth decimal for $n = 5, ..., 9$. It is also clear that all these eigenvalues are doubly degenerate, at least up to four decimals.

We made a plot of the ground state eigenfunction of $\tilde{H}_N$ as well. This function has been compared to the ground state of J_{N+1}/N. Both graphs are displayed in Figure 4.5.

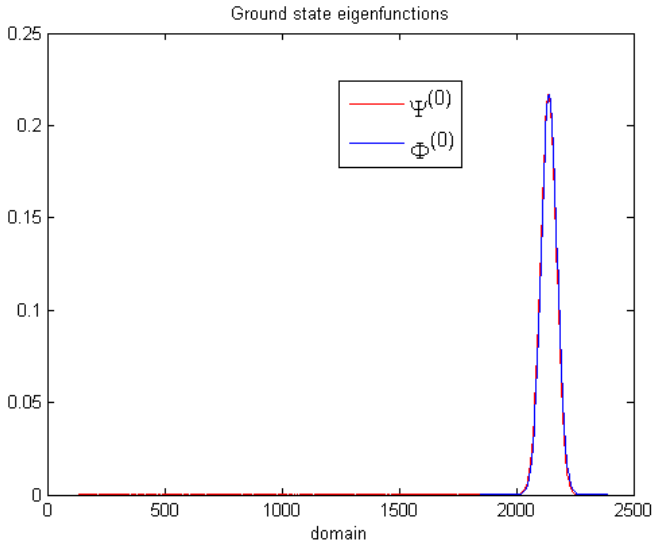

Figure 4.5: Both ground states plotted on the domain of order N, for N=1000. $\Psi^{(0)}$ corresponds to $\tilde{H}_N$ and $\Phi^{(0)}$ to J_{N+1}/N.

In fact, since the ground state is already numerically doubly degenerate for $N = 1000$, the computer picks a linear combination of the two eigenvectors, as already explained in §3.2. This choice is kind of random, since when one changes N, the computer might pick the left located peak as a ground state as well. We forced the computer to take the right located peak for both operators in order to compare. The table and the graph above show, at least numerically, that we have strong evidence that the original tridiagonal matrix may is related to $\tilde{H}_N$. This is a priori not directly clear since J_{N+1}/N only contains two equal sub-blocks that approximate the sub-block of order $\sqrt{N}$ in the matrix $\tilde{H}_N$, given by

$$-\frac{1}{8}\,[\cdots 1\ \ -2\ 1\cdots] + \mathrm{diag}(J_{N+1}/N) - \frac{1}{4}. \tag{4.85}$$

The reason for this strong (numerical) result probably lies in the fact that the eigenvectors of both operators *only* localize on the specific subset of order $\sqrt{N}$, centered around the two minima of the well.[11]

We have computed the minimum of the potential, set it to zero, and subtracted this minimum from the lowest eigenvalues. Then, these shifted eigenvalues live in a positive potential with minimum equal to zero. For J_{N+1}/N and $N = 1000$, we now consider the eigenvalues ϵ_n of this matrix. We have already seen above that the lowest eigenvalues of J_{N+1}/N become doubly degenerate. Therefore, we identify these approximately doubly degenerate eigenstates with one single state that we denote by n. It follows that each n corresponds to two (approximately) degenerate eigenvalues, e.g., $n = 0$ corresponds to the ground state as well as the first excited state of J_{N+1}/N, $n = 1$ corresponds to the second and the third excited state, and so on. This is displayed in the table below.

[11] This has been numerically checked in §4.5, see for example Figure 4.1.

Shifted eigenvalues for odd values of n	
n	ϵ_n
0	0.000863
1	0.002591
2	0.004310
3	0.006013
4	0.007710

Using this table, we deduce that the energy splitting is given approximately given by $\sqrt{3}/N$, when N large enough. The ground state (shifted) eigenvalue (which is approximately doubly degenerate) is then given by $\frac{1/2\sqrt{3}}{N}$, the first excited state (also approximately doubly degenerate) by $\frac{3/2\sqrt{3}}{N}$, the second excited state by $\frac{5/2\sqrt{3}}{N}$ etc. Therefore, there is excellent numerical evidence that the (approximately) doubly degenerate shifted spectrum of J_{N+1}/N is given by

$$\frac{(n+1/2)\sqrt{3}}{N}, \quad \text{for } N \text{ large enough.} \tag{4.86}$$

Note that the eigenvalues for $N = \infty$ appear to be all zero, and we will see in the next paragraph that these are not even defined in this case. Moreover, observe that the values in both tables are computed for fixed N. Therefore, also different values of N need to be considered. We will focus on the ground state eigenvalue ϵ_0^N of the matrix J_{N+1}/N. See the table below.

$N\epsilon_0^N$ for increasing N	
N	$N\epsilon_0^N$
100	0.8473
1000	0.8633
2500	0.8653
5000	0.8655

Thus ϵ_0^N will approximate $\frac{1/2\sqrt{3}}{N}$ when N increases. This shows that (4.86) indeed makes sense.

What do we learn from these simulations?
We started with the tridiagonal matrix J_{N+1}/N. Using a central difference approximation on a non-uniform grid, we showed that locally we had (an approximate) uniform discretization precisely on a subset of order $\sqrt{N}$ centered around the maxima of the Gaussian-like ground state peaks. Therefore, locally, this matrix approximates a kinetic and a potential energy, meaning that there exists a sub-block in the matrix J_{N+1}/N that has the form approximately given by $T + V$, as we explained in detail before. Using this fact, we constructed the matrix $\tilde{H}_N$. In fact, we showed that J_{N+1}/N locally approximates $\tilde{H}_N$. This in turn means that J_{N+1}/N applied to those vectors living on a specific subset on which the discretization was uniform, and are zero outside this set, yields the same vectors as $\tilde{H}_N$ applied to these vectors. We have seen that this set was centered around the maxima of the Gaussian-shaped ground state eigenvectors. In the construction of $\tilde{H}_N$ we computed the potential $\tilde{V}_N$ that had the shape like a double well. We found that the maxima of the doubly peaked Gaussian ground state correspond precisely with the minima of a potential well. Moreover, we have convincing numerical evidence that J_{N+1}/N is related to $\tilde{H}_N$, since also their spectral properties coincide to very good approximation. If N increases, this approximation gets better. The spectral properties of $\tilde{H}_N$ behave like a Schrödinger operator describing a particle in a symmetric double well. This lead us to the surmize that $\tilde{H}_N$ is the discretization of a Schrödinger operator. In §4.7 we give the precise connection between $\tilde{H}_N$ and the Schrödinger operator $\tilde{h}_2$ on $L^2([0,1])$. Since J_{N+1} is in turn related to $\tilde{H}_N$, we first say something more about these matrices. This will be the final part of this paragraph.

For each finite N the matrix $\tilde{H}_N$ is a finite-dimensional tridiagonal matrix, which can be identified with an element of $B(\ell^2_N(\mathbb{N}))$, where the latter space is the space of linear operators on the Hilbert space of all finite sequences of length N. It is easy to see that the coefficients of $\tilde{H}_N$ are bounded when $N \to \infty$ and $0 \leqslant j \leqslant N$. Moreover, for each $N \in \mathbb{N}$, the off-diagonal entries of $\tilde{H}_N$ have the same sign. Therefore, one might expect that in the limit the matrix will be bounded as well. Moreover, since for each finite N the matrix is self-adjoint, one might expect the same result in the limit. The same result holds for J_{N+1}/N. Therefore, one could try to prove that both matrices converge to so-called bounded self-adjoint Jacobi operators on $\ell^2(\mathbb{N})$. Based on the similar spectral properties of both matrices, one could expect that that there exists a unitary operator u_{N+1} such that $\tilde{H}_{N+1}$ and J_{N+1}/N become asymptotically unitary equivalent, in that:

$$\lim_{N\to\infty} ||u_{N+1}\tilde{H}_{N+1}u^*_{N+1} - J_{N+1}/N||_{N+1} = 0. \tag{4.87}$$

Note that the operator norm depends on N as well and does not converge in general. The above conjecture is not easy to prove, as it is purely based on numerical results. Furthermore, it is not relevant what this limit will be, since we only have to consider finite N in the semiclassical limit, as we will see soon. In any case, we have strong evidence that there is a relation between the matrices J_{N+1}/N and $\tilde{H}_{N+1}$ that might be given by the above formula.

4.7 Link with a Schrödinger operator on $L^2([0,1])$

In this section, we are first going to make a link between the matrix $\tilde{H}_N$ and a Schrödinger operator on a domain of order N, viewed as a subset of $L^2(\mathbb{R})$. We denote this operator by $\tilde{h}_1$. Then we scale $\tilde{h}_1$ to an operator defined on $L^2([0,1])$, which we denote by $\tilde{h}_2$. This operator is the one we mentioned in the beginning of §4.6, viz. (4.72). We should remark that the fixed values of $B = 1/2$ and $J = 1$ used in the matrix entries for J_{N+1}/N determine also $\tilde{H}_N$ and hence $\tilde{h}_2$. Thus, the results derived in this section are based on these two parameters.

In §4.5 we explained how to approximate a second order differential operator with a discretization matrix using a central difference scheme. We also showed that a symmetric tridiagonal matrix with constant off- and diagonal entries can be identified with a discretization of a Schrödinger operator on a uniform grid. We now apply this procedure to the matrix $\tilde{H}_N$ and we are going to find the corresponding Schrödinger operator that we denoted by $\tilde{h}_1$. The matrix $\tilde{H}_N$ corresponds to a uniform grid spacing of $\sqrt{8}$ on a grid of length $\sqrt{8}N$. Applying the method explained in §4.5, it follows that we can identify $\tilde{H}_N$ with the sum of a second order derivative $\frac{d^2}{dx^2}$ and a multiplication operator $m_{\tilde{V}_N}$ acting on the space $L^2([0, L_N])$:

$$\tilde{h}_1 = -\frac{d^2}{dx^2} + m_{\tilde{V}_N}. \tag{4.88}$$

Here, $m_{\tilde{V}_N}$ is the operator that acts as multiplication by $\tilde{V}_N$. It is the continuous analog of the matrix (4.83), but note that its domain still depends on N. The constant L_N denotes the length of the interval which equals $\sqrt{8}N$. $\tilde{h}_1$ is of course an unbounded operator. It is not clear how the operator $\tilde{h}_1$ behaves when N increases, since the domain increases with N and so the potential minima of $\tilde{V}_N$ as well. Therefore, we will scale the interval by its length L_N, so that it becomes fixed. Thus scaling this interval by its length gives an operator on an interval of order 1. We denote this operator by $\tilde{h}_2$. Note that the variable $y \in [0,1]$ satisfies $y = x/L_N$, so that $dx/dy = L_N$, and hence $d/dx = \frac{1}{L_N} d/dy$. The Schrödinger operator on the unit interval is therefore given by

$$\tilde{h}_2 = -C_N \frac{1}{8}\frac{d^2}{dy^2} + m_{\tilde{V}}, \tag{4.89}$$

with $C_N = N^{-2}$. The potential $\tilde{V}$ (for $B = 1/2$ and $J = 1$) is then given by the continuous function

$$\tilde{V}(y) \approx -\frac{1}{2}(2y-1)^2 - \sqrt{(1-y)y}, \quad y \in [0,1]. \tag{4.90}$$

As we have explained in the beginning of the previous paragraph, it is clear that for $\hbar = 1/N$, we recognize the well-known Schrödinger operator describing a particle in a symmetric double well potential. We will see in §6.3 that a far more sophisticated deformation quantization is needed to pass from quantum mechanics ($\hbar > 0$) to classical mechanics ($\hbar = 0$).

It is also clear that $\tilde{H}_N$ is a correct discretization of $\tilde{h}_2$: a matrix of dimension N on an interval of order 1 gives a grid spacing $\Delta = 1/N$. It follows that

$$-\frac{1}{8N^2}\frac{d^2}{dy^2} \approx -\frac{1}{8N^2}\frac{[\cdots 1 \ -2 \ 1 \cdots]_N}{\Delta^2} = -\frac{1}{8}[\cdots 1 \ -2 \ 1 \cdots]_N, \tag{4.91}$$

and the latter matrix is precisely $\tilde{T}_N$ from $\tilde{H}_N$.
Thus, a claim/conclusion that connects these operators is the following[12]:

Claim 4.7.1. *The matrix $\tilde{H}_N$ defined by* (4.69) *is a discretization of the Schrödinger operator $\tilde{h}_2$ on an interval of order 1. The term 'discretization' refers to the one given by* (4.91)*.*

We have seen in the previous paragraph that the approximation $\tilde{H}_N$ by J_{N+1}/N gets better with increasing N, so that one should consider $\tilde{H}_N$ and thus $\tilde{h}_2$ for large N.

Remark. When one would start with a Schrodinger operator on some interval, then one should beware of the following. Discretizing an operator on a finite grid means restricting the original operator to some subspace and projecting this restricted operator onto that subspace. One can take a basis for this subspace, and writing the operator with respect to this basis gives a finite dimensional matrix. This matrix, then, will be a discretized analog of the original operator. This result of course strongly depends on the subspace and the basis.

In our case, we have linked $\tilde{H}_N$ to a Schrodinger operator on $L^2([0,1])$. We have argued that the matrix $[\cdots 1 \ -2 \ 1 \cdots]_N$ corresponds to the second order derivative operator $-C_N d^2/dy^2$ on an interval of order 1. In view of the above remark, there exists some finite-dimensional subspace and a basis, so that its corresponding matrix is indeed of that specific form. However, finding this subspace and basis is not really relevant anymore since we are given the discrete matrix $\tilde{H}_N$, from which we derived a Schrödinger operator.

It is well known that the ground state of the operator $\tilde{h}_2$ for finite N looks approximately like a doubly peaked Gaussian, where each peak is centered in one of the minima of the potential. For infinite N, these peaks will behave like delta peaks, but they are not eigenfunction anymore since $\tilde{H}_2$ is not defined for $N = \infty$ [34], [22, Sec. 10.1,10.2].
Moreover, numerical simulations (Figure 4.1) show that the eigenfunctions of $\tilde{H}_N$ live approximately on a grid of order $\sqrt{N}$ points on he interval $[0,1]$. Using the above discretization, we then have an order $\sqrt{N}$ steps of $1/N$ each, so that in particular the ground state Gaussian has a width of $1/\sqrt{N}$. On the one hand, it is clear that this width will go to zero as $N \to \infty$. On the other hand, also the unit interval depends on N, as the latter has to be discretized with $N+1$ points. The grid spacing of $1/N$ will go to zero when $N \to \infty$ too. Therefore, the total number of points in the ground state

[12] Note that this claim is based on the fact that the number N occuring in the factor $1/N$ in front of the derivative $\frac{d^2}{dy^2}$ in (4.91) is the same as the dimension of the discretization matrix $[\cdots 1 \ -2 \ 1 \cdots]_N$.

peak living on a subset of order $\sqrt{N}$ is given by

$$\frac{1/\sqrt{N}}{1/N} = \sqrt{N} \tag{4.92}$$

Even though the ground state will behave like a delta peak when N gets larger, when discretizing the grid, the number of points in this peak increases with $\sqrt{N}$. In fact, due to the discretization of the grid we have a better approximation of the Gaussian ground state when N increases.

The equivalence between J_{N+1}/N and $\tilde{H}_{N+1}$ for N large was originally obtained from a discretization based on a central difference scheme using a non-uniform grid. Moreover, we have seen that the operator $\tilde{H}_{N+1}$ can be linked to a Schrödinger operator on $L^2([0,1])$.
Consider now this Schrödinger operator $\tilde{h}_2$. For convenience, one can identify C_N with $\hbar^2$, for $\hbar = 1/N$ small, so that the operator under this identification is given by

$$\tilde{h}_2 = -\frac{\hbar^2}{8}\frac{d^2}{dx^2} + V(x). \tag{4.93}$$

It is also known (see e.g., §4.8 or [12], [14]) that the lowest eigenstates of such a Schrödinger operator are approximately degenerate when the barrier of the double well potential is sufficiently high enough. For such a potential, we have seen that these states approximately behave like a linear combination of weighted Hermite polynomials centered in both minima of the potential. These polynomials are in general given by

$$\varphi_n(x) = e^{-x^2/2}H_n(x), \qquad n = 0, 1, 2, ... \tag{4.94}$$

Thus for this type of potential, the ground state in particular is approximately given by two Gaussians, each localized in one of the minima. The spectrum of this operator consists of eigenvalues and the lowest eigenvalues are approximately doubly degenerate and equidistant in this semiclassical approach. This relies on the assumption that we can approximate both wells with a parabola (see §4.8 for a justification of this assumption).

It can then be shown that the eigenvalues of $\tilde{h}_2$ are approximately given by

$$E_{n,\pm} \approx (n + 1/2)\hbar\omega \mp \hbar C e^{-\frac{1}{\hbar}\varphi}, \quad (n = 0, 1, 2...). \tag{4.95}$$

where φ an integral with positive integrand, and $C > 0$. In the case for $\tilde{h}_2$, we have a factor $1/N$ which now plays the role of $\hbar$ in (4.93). Hence, as expected, we find that also now $e^{-N\varphi} \approx 0$, if N large. As a result, the lowest eigenstates indeed become approximately doubly degenerate as we have already seen from the tables in §4.6. We will give a detailed analysis in §4.8.

We conclude this paragraph by recalling the following statement.
The most important property linking the quantum Curie-Weiss model to a Schrödinger operator is the existence of a subspace, namely $\mathrm{Sym}^N(\mathbb{C}^2)$, so that the matrix representation of the operator h_N^{CW} restricted to this subspace became a tridiagonal matrix J_{N+1}/N that could be seen as a discretiation $\tilde{H}_{N+1}$ of a Schrödinger operator $\tilde{h}_2$. One should still prove the correct asymptotic equivalence between this matrix J_{N+1}/N, and the matrix $\tilde{H}_{N+1}$, for N large, but finite. This then, in combination with Theorem (4.7.1), should really prove a semi-classical equivalence between J_{N+1}/N and the Schrödinger operator $\tilde{h}_2$. Unfortunately, we were not able to prove this mathematically.

4.8 Double well with WKB

In the previous paragraph, we have argued that we can view our matrix J_{N+1}/N as a discretization $\tilde{H}_N$ of the Schrödinger operator $\tilde{H}_2$, when N sufficiently large. We have already mentioned some properties about the spectrum and the lowest eigenstates corresponding to this Schrödinger operator.
In this section we use the WKB-approximation method applied to a double well potential to deduce these results. Most of the work done in this section is based on [34]. We consider the following situation, displayed in Figure 4.6.

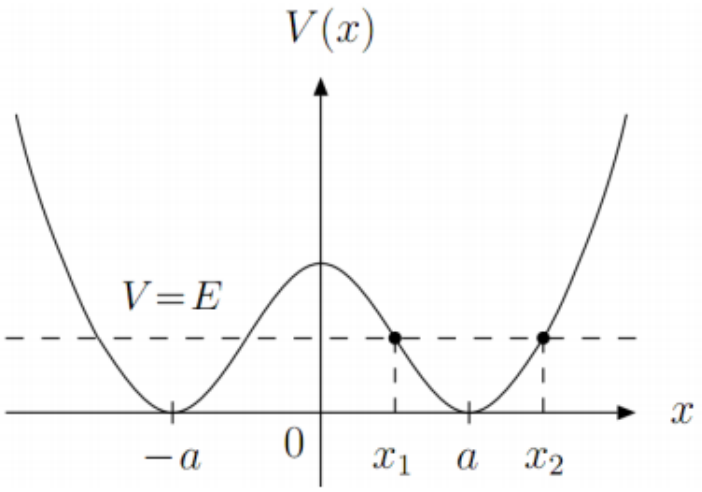

Figure 4.6: Symmetric double well with turning points $\pm x_1$ and $\pm x_2$ and minima $\pm a$. The figure is taken from [34].

We are going to determine the energy levels below the potential, i.e., the energies for which $E < V(0)$ holds. From the results obtained in Appendix C, it can be shown that the wave function for this classical forbidden area $(-x_1 < x < x_1)$, below the potential, takes the following form:

$$\psi^{\mathrm{WKB}}(x) \simeq \frac{D}{\sqrt{|p(x)|}}\left[2\cos\theta \exp\left(\frac{1}{\hbar}\int_x^{x_1} |p(x')|dx'\right) + \sin\theta \exp\left(-\frac{1}{\hbar}\int_x^{x_1} |p(x')|dx'\right)\right], \tag{4.96}$$

where $-x_1 \leqslant x < x_1$. Here, D is the coefficient corresponding to the WKB solution on the interval (x_2, ∞).
Since the potential is symmetric, it commutes with the parity operator. Moreover, the energy levels in the potential well are non-degenerate, as we will see in Chapter 5. Thus, we automatically have that the energy eigenfunctions need to be parity eigenfunctions. Hence we only need to consider the even ψ_+^{WKB} and odd ψ_-^{WKB} wave functions. In the former case $\frac{d}{dx}\psi_+^{\mathrm{WKB}}(0) = 0$, and in the latter case $\psi_-^{\mathrm{WKB}}(0) = 0$. For the antisymmetric (odd) case, the property $\psi_-^{\mathrm{WKB}}(0) = 0$ implies that

$$\frac{D}{\sqrt{|p(x)|}}\left[2\cos\theta \exp\left(\frac{1}{\hbar}\int_0^{x_1} |p(x')|dx'\right) + \sin\theta \exp\left(-\frac{1}{\hbar}\int_0^{x_1} |p(x')|dx'\right)\right] = 0, \tag{4.97}$$

which in turn implies

$$\begin{aligned}\tan\theta &= -2e^{-\frac{2}{\hbar}\int_0^{x_1}|p(x')|dx'} \\ &= -2e^{-\frac{1}{\hbar}\int_{-x_1}^{x_1}|p(x')|dx'} \\ &= -2e^{-\phi},\end{aligned} \tag{4.98}$$

where we used the fact that p is even, as well as

$$\phi = \frac{1}{\hbar}\int_{-x_1}^{x_1}|p(x')|dx'. \tag{4.99}$$

For the symmetric (even) case , we have $\psi(x_1) = \psi(-x_1)$, so that we find

$$\frac{D}{\sqrt{|p|}}(\sin\theta + 2\cos\theta) = \frac{D}{\sqrt{|p|}}(\sin\theta e^{-\frac{1}{\hbar}\int_{-x_1}^{x_1}|p(x')|dx'} + 2\cos\theta e^{\frac{1}{\hbar}\int_{-x_1}^{x_1}|p(x')|dx'}), \tag{4.100}$$

which by definition implies

$$\frac{D}{\sqrt{|p|}}\bigg(\sin\theta + 2\cos\theta\bigg) = \frac{D}{\sqrt{|p|}}\bigg(\sin\theta e^{-\phi} + 2\cos\theta e^{\phi}\bigg). \tag{4.101}$$

Hence

$$\begin{aligned}\tan\theta &= 2\frac{1-e^{-\phi}}{e^{-\phi}-e^{-2\phi}} \\ &= 2e^{-\phi}.\end{aligned} \tag{4.102}$$

From this we conclude that

$$e^{-\phi} = \frac{\pm 2}{\tan\theta}. \tag{4.103}$$

Solving these equations exactly is not possible analytically in most cases,. If we assume that the potential barrier is very high and broad, we we can get an idea of the general behaviour of the system. Since ϕ, which is the integral over the magnitude of imaginary momentum and represents the phase, is going to very large in such a case, it follows that $e^{-\phi}$ is very small. Therefore, by definition of the tangent function, θ must be very close to $(n+\frac{1}{2})\pi$. With this in mind, let us write $\theta = (n+\frac{1}{2})\pi + \epsilon$, where $\epsilon << 1$. Then it follows that:

$$\begin{aligned}&\tan(n+\frac{1}{2})\pi + \epsilon \approx \pm 2e^{\phi} \\ \implies &\cot(-n\pi - \epsilon) \approx \pm 2e^{\phi} \\ \implies &-\cot\epsilon \approx \pm 2e^{\phi} \\ \implies &\frac{1}{\epsilon} \approx \mp 2e^{\phi} \\ \implies &\epsilon \approx \mp\frac{1}{2}2e^{-\phi}.\end{aligned} \tag{4.104}$$

Thus the quantization condition simplifies to

$$\theta \approx (n+\frac{1}{2})\pi \mp \frac{1}{2}e^{-\phi}. \tag{4.105}$$

In a first approximation, we see immediately that

$$\theta = (n+\frac{1}{2})\pi. \tag{4.106}$$

This can also be understood since tunneling through a very high and broad barrier is almost impossible, and hence the physically particle will be localized in one of the two wells. In this case, we know that the allowed energies correspond to those of a single well potential, for which the quantization condition is precisely given by (4.106) [2]. In this case, both the even and the odd wave function have the corresponding energy level of the single well potential, which we denote by $E_n^{(0)}$ $(n = 0, 1, 2, ...)$. For the harmonic oscillator in a single well, these energies are given by $E_n^{(0)} = (n + 1/2)\hbar\omega$. For a double well with a high and broad barrier, it therefore makes sense to write

$$E_{n,\pm}^{\mathrm{WKB}} = E_n^{(0)} + \Delta E_{n,\pm} \quad (n = 0, 1, 2, ...), \tag{4.107}$$

where $\Delta E_{n,\pm}$ is assumed to be much smaller than $E_n^{(0)}$.[13]

The next step is to find an expression for the energy splitting of the ground state $\Delta E_{0,\pm}$. Again, we assume that the potential barrier is very high and broad, and suppose that $\psi_0^{(0)}$ is the WKB wave function corresponding to the ground state in the classical forbidden region $(-x_1 < x_1)$, located in the right well. This corresponds to (C.17), for $D = 0$. Then, we may write

$$\psi_0^{(0)}(x) \simeq \frac{C}{\sqrt{|p(x)|}} \exp\left(\frac{1}{\hbar}\int_0^x |p(x')|dx'\right). \tag{4.108}$$

We can compute its derivative. It follows by the chain rule that

$$\psi_0^{(0)\prime}(x) \simeq \left(\frac{|p(x)|}{\hbar} - \left|\frac{p'(x)}{2p(x)}\right|\right)\psi_0^{(0)}(x) \approx \frac{|p(x)|}{\hbar}\psi_0^{(0)}(x), \tag{4.109}$$

where we neglect the second term, since we assume that the system is in a semi-classical state for which (C.14) holds. We then use Herring's formula[14] for an expression for the energy splitting $\Delta E_{n,\pm}$ in terms of $\psi_n^{(0)}$:

$$\Delta E_{n,\pm} = \mp\frac{\hbar^2}{2m}\psi_n^{(0)}(0)\psi_n^{(0)\prime}(0). \tag{4.110}$$

Using Herring's formula and (4.108), it follows that

$$\Delta E_{0,\pm} = \mp\frac{\hbar}{m}C^2. \tag{4.111}$$

Thus, our task is to determine C. First we make another assumption. We assume that the potential V in the area (x_1, x_2) can be approximated by a quadratic potential in a neighborhood of its minimum at $x = a$, like the case of a harmonic oscillator. Since we focus on the area (x_1, x_2), we consider

$$V(x) \approx \frac{1}{2}m\omega_0^2(x - a)^2, \tag{4.112}$$

where the constant ω_0 is given by $\omega_0 = \sqrt{V''(a)/m}$, with a the position of the minimum of the well on the right site, and V the original potential.

[13] We will soon see that this is indeed the case for the ground state energy splitting $\Delta E_{0,\pm}$.

[14] This formula is named after Herring, who derived it in the analysis of a problem relating the H_2^+ molecular ion [15], [16].

Assuming (4.112), this implies that both the ground state wave function and the ground state energy match those of the harmonic oscillator:

$$E_0^{(0)} \approx \frac{1}{2}\hbar\omega_0, \tag{4.113}$$

$$\psi_0^{(0)}(x) \approx \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega_0}{2\hbar}(x-a)^2}. \tag{4.114}$$

We also assume that this approximation of the wave functions is valid in the whole region $(-x_1, x_1)$. Then, in order to determine C, we have to compare (4.108) and (4.114). Therefore, we need to compute $|p(x)|$ in the region $(-x_1, x_1)$. Using $V(x_1) = E_0^{(0)}$, we compute

$$\begin{aligned} |p(x)| &= \sqrt{2m\Big(V(x) - E_0^{(0)}\Big)} \\ &= \sqrt{2m\Big(V(x) - V(x_1)\Big)} \\ &= m\omega_0\Big((a-x)^2 - (a-x_1)^2\Big)^{1/2}. \end{aligned} \tag{4.115}$$

Now, we define $y_0 \equiv a - x_1$. Again using $V(x_1) = E_0^{(0)}$, it follows that y_0 is approximately equal to

$$y_0 \approx \sqrt{\frac{\hbar}{m\omega_0}}. \tag{4.116}$$

For a barrier that is sufficiently high and broad, we may neglect the term y_0^2 in computing $|p(x)|$ for the ground state on $(-x_1, x_1)$, since on this interval we have $a - x >> a - x_1$. It follows that

$$\psi_0^{(0)}(x) \simeq \frac{C}{\sqrt{m\omega_0(a-x)}} \exp\left(\frac{1}{\hbar}\int_0^{x_1} |p(y)|dy + \Phi(x)\right), \tag{4.117}$$

where Φ is given by

$$\Phi(x) = -\frac{1}{\hbar}\int_x^{x_1} |p(y)|dy \tag{4.118}$$

$$= -\frac{m\omega_0}{\hbar}\int_x^{x_1} [(a-y)^2 - (a-x_1)^2]^{1/2} dy \tag{4.119}$$

$$\approx -\frac{m\omega_0(a-x)^2}{2\hbar} + \frac{1}{2}\log\left(\frac{2(a-x)}{y_0}\right) + \frac{1}{4} + O\left(\frac{y_0^2}{(a-x)^2}\right). \tag{4.120}$$

Comparing (4.108) with (4.117), it follows that

$$C = \left(\frac{m^2\omega_0^2}{4\pi e}\right)^{1/4} e^{-\frac{1}{\hbar}\int_0^{x_1} |p(y)|dy}. \tag{4.121}$$

Then formula (4.111) reads

$$\Delta E_{0,\pm} = \mp\frac{\hbar\omega_0}{2\sqrt{\pi e}} \exp\left(-\frac{1}{\hbar}\int_{-x_1}^{x_1} \sqrt{2m[V(y) - E_0^{(0)}]}dy\right). \tag{4.122}$$

This procedure can also be applied for higher energy levels. All one needs to do is match the WKB wave function in the classically forbidden region $(-x_1, x_1)$ to the n^{th} harmonic oscillator state and

use Herring's formula to find $\Delta E_{n,\pm}$. We can also see that the splitting becomes large if the energy increases or the barrier decreases in height and width, since the integral in the last expression decreases in that case. The energy splitting will disappear for a very high and broad barrier.

Now, we are going to compute the lowest eigenenergies numerically using the formula we have just derived. We take the double well potential corresponding to the Schrödinger operator $\tilde{h}_2$ on $L^2([0,1])$, as derived in §4.7. Still keep in mind that this operator is derived from the matrix J_{N+1}/N for $B = 1/2$ and $J = 1$. For N large enough, we could approximate the potential by a continuous function, in that

$$\tilde{V}(y) \approx -\frac{1}{2}(2y-1)^2 - \sqrt{(1-y)y}, \quad y \in [0,1]. \tag{4.123}$$

We have to determine the minima a and the mass m in order to compute $\omega \equiv \sqrt{\frac{V(''(a)}{m}}$. We have already seen that the minimum of the above potential is attained at $x = 1/2 \pm 1/2\sqrt{3}$. This can be easily shown by computing the derivative. It is also elementary to show that the second derivative of the above function equals

$$V''(y) = \frac{1}{4(-(y-1)y)^{3/2}} - 4, \tag{4.124}$$

so that $V''(\pm a) = 12$. As we have seen, we put $\hbar = 1/N$ in (4.93). In order to find the mass, we compare the factor $\frac{1}{8}$ in $\tilde{h}_2$ from (4.89) with the factor in front of the derivative in (4.93). We see that $m = 4$. It follows that $\omega_0 = \sqrt{\frac{V''(a)}{m}} = \sqrt{\frac{12}{4}} = \sqrt{3}$. Thus $\hbar\omega_0 = \sqrt{3}/N$.

Now, consider the formula we derived before,

$$E^{\mathrm{WKB}}_{n,\pm} = (n+1/2)\hbar\omega_0 + \Delta E_{n,\pm}, \quad (n = 0,1,2,...) \tag{4.125}$$

where $\omega_0 = \sqrt{3}$ and $\Delta E_{n,\pm}$ given by (4.122). We compare it to the lowest eigenenergies of the operator $\tilde{H}_N$, which was a discretization of the Schrödinger operator $\tilde{h}_2$. It is immediately clear that the first term $(n+1/2)\hbar\omega_0$ equals $\frac{(n+1/2)\sqrt{3}}{N}$, exactly as we found before. In order to compute the second term $\Delta E_{n,\pm}$, we compute

$$\begin{aligned}
-\frac{1}{\hbar}\int_{-x_1}^{x_1}\sqrt{2m[V(x') - E_0^{(0)}]}dx' &= -\frac{1}{\hbar}\int_{-x_1}^{x_1} m\omega_0[(a-x')^2 - (a-x_1)^2]^{1/2}dx' \\
&= -\frac{2m\omega_0}{\hbar}\int_0^{x_1}[(a-x')^2 - (a-x_1)^2]^{1/2}dx' \\
&= \frac{2m\omega_0}{\hbar}\int_a^{y_0}[y^2 - y_0^2]^{1/2}dy \\
&= \frac{2m\omega_0}{\hbar}\frac{1}{2}\left(y\sqrt{y^2-y_0^2} - y_0^2\log\left(y + \sqrt{y^2-y_0^2}\right)\right)_a^{y_0} \\
&= \frac{m\omega_0}{\hbar}\left[\left(-a\sqrt{a^2-y_0^2} + y_0^2\log\left(a + \sqrt{a^2-y_0^2}\right)\right) - y_0^2\log y_0\right].
\end{aligned} \tag{4.126}$$

Since we assume that $y_0 \approx \sqrt{\frac{\hbar}{m\omega_0}}$, and m, ω_0 and a are parameters from the potential, we are able to compute the above equation, and hence the WKB-ground state energy $E^{\mathrm{WKB}}_{0,\pm}$. For these parameters, we find that (4.126) equals

$$-\frac{1}{\hbar}\int_{-x_1}^{x_1}\sqrt{2m[V(x') - E_0^{(0)}]}dx' \approx -\frac{6}{\hbar} = -6N. \tag{4.127}$$

Moreover, note that the prefactor $\frac{\hbar\omega_0}{2\sqrt{\pi e}}$ in (4.122) for our parameters is approximately equal to

$$\frac{\hbar\omega_0}{2\sqrt{\pi e}} \approx 0.296/N. \tag{4.128}$$

As $|p(x)| = \sqrt{2m[V(x') - E_0^{(0)}]}$ is positive, the exponential of the equation (4.126) is bounded by 1. Thus, we know that

$$\Delta E_{0,\pm} \leqslant \frac{\hbar\omega_0}{2\sqrt{\pi e}} \approx 0.296/N. \tag{4.129}$$

We see that for N sufficiently large, the ground state energy splitting is about zero. In fact, it goes even faster to zero since we have to take the exponential factor into account as well. It follows that the ground state energy splitting for our potential behaves like

$$\Delta E_{0,\cdot\pm} \approx \mp\frac{0.296}{N} e^{-6N}. \tag{4.130}$$

Even for $N = 1$, the above equation is already in the order 10^{-4}.

We give a summary.
We have seen that for increasing but finite N, the spectrum of the operator J_{N+1}/N approximates the one of the matrix $\tilde{H}_N$, playing the role of a discretization of the Schrödinger operator $\tilde{h}_2$. For $N = 1000$, the (shifted) ground state of the operator J_{N+1}/N was, up to five decimals, equal to the number $0.8633/N$. For this relative large value of N, this number was the same as the (shifted) ground state eigenvalue corresponding to $\tilde{H}_N$ (see tables in §4.6). If one compares this number to (4.125) (for $n = 0$ in (4.122)) derived from the WKB-approximation for $N = 1000$, then it is clear that for this value of N, to a very good approximation both energy levels are completely degenerate, and are given by $\frac{\sqrt{3}}{2N}$. On the one hand, the approximation of $\tilde{H}_N$ by J_{N+1}/N gets better for relative large values of N, and we have seen that the ground state eigenvalue becomes numerically two-fold degenerate, already for $N \approx 80$. For these and larger values of N, the energy splitting (4.122) has been computed and and is of order $< 10^{-200}$. Accordingly, it is reasonable to speak about a degenerate ground state as we indeed have observed numerically. Moreover for $N = 80$, the shifted ground state eigenvalue is approximately given by $0.842/N$. On the other hand, the value of $N = 80$ is still relatively small when one wants to give a better approximation of $\frac{\sqrt{3}}{2N} \approx 0.866$, even though the ground state may be numerically degenerate. In order to find a better approximation of $\frac{\sqrt{3}}{2N}$, one should increase N much more. Note that for values of $N < 80$, we have seen that the energy levels of J_{N+1}/N are non-degenerate. In this regime the WKB-approximation is definitely not applicable, since for say $N = 60$, according to this approximation the energy splitting is already in the order of 10^{-160}, so that we may speak about degenerate eigenvalues, even though we know that the eigenvalues of J_{N+1}/N of $\tilde{H}_N$ are not degenerate.

Therefore, applied to our double well potential, the WKB approximation does not match one to one for the value of $\hbar = 1/N$. It can only be used as an indication of the energy *splitting* of the lowest eigenenergies, not as a quantitative tool to predict the absolute values of the eigenenergies.

Chapter 5

Perron-Frobenius Theorem

In this section we provide machinery in order to prove the Perron-Frobenius Theorem, in finite and infinite dimensions. First, we discuss a version of the Perron-Frobenius Theorem in the setting of linear algebra, i.e. we state this theorem for matrices. Then, we give an overview and a prove an important theorem that extends the Perron-Frobenius Theorem in infinite dimensions. Moreover, we apply this theorem to the N-dimensional spin system given by the Curie-Weiss Hamiltonian. Finally, we will apply it to some class of Schrodinger operators, since we have seen in Chapter 4 that these play an important role as continuous analog of our scaled Curie-Weiss Hamiltonian, represented with respect to the canonical base for $\mathrm{sym}^N(\mathbb{C}^2)$.

5.1 Perron-Frobenius theorem for N-dimensional matrices

We start with some definitions and basis facts.

Definition 5.1. *A square matrix is called non-negative if all its entries are non-negative. It is called strictly positive if all its entries are strictly positive.*

Definition 5.2. *A non-negative matrix a is called irreducible if for every pair indices i and j there exists a natural number m such that $(a^m)_{ij}$ is not equal to zero. If the matrix is not irreducible, it is said to be reducible.*

Definition 5.3. *A directed graph is a graph $G = (V, E)$ with vertices V and edges E such that the vertices are connected by the edges, and where the edges have a direction. A directed graph is also called a digraph.*

Definition 5.4. *A digraph is called strongly connected if there is a directed path x to y between any two vertices x, y.*

We use the notion of the directed graph or digraph of a square N-dimensional matrix a, denoted by $G(a)$. We say that the digraph of a is the digraph with

$$V = \{1, 2, ..., N\},$$
$$E = \{(i, j)|\ a_{ij} \neq 0\}.$$

There is a relation between irreducibility of a matrix and connectedness of the corresponding digraph:[1]

Lemma 5.5. *A non-negative matrix square a is called irreducible if and only if the digraph of a is strongly connected.*

[1]These basis facts are take from **www.transo.com.tw/shwu/note/AMN_07.ppt**

Proof. $\Rightarrow$) Given a square non-negative matrix a, and $m \in \mathbb{N}_+$. If $(a^m)_{ij} \neq 0$ for some pair (i,j), then there exists a direct path in $G(a)$ of length m from vertex i to vertex j. Compute, using matrix multiplication:

$$(a^m)_{ij} = \sum_{1 \leqslant i_2 \leqslant \ldots \leqslant i_m} a_{ii_2} a_{i_2 i_3} \cdots a_{i_m j}. \tag{5.1}$$

If $(a^m)_{ij} \neq 0$, then there exists $1 \leqslant i_2, i_3, ..., i_m \leqslant m$ such that $a_{ii_2} \cdot a_{i_2 i_3} \cdots a_{i_m j} \neq 0$. Hence $(i,i_2),(i_2,i_3),...,(i_m,j) \in E$. Thus there is a direct path of length m from vertex i to vertex j. This is precisely the definition of a strongly connected digraph. Hence irreducibility of a implies that the digraph of a is strongly connected.

$\Leftarrow$) Assume that a is reducible. Then the set of vertices V can be partitioned into two non-empty sets V_1 and V_2 in such a way that there is no path from any vertex in V_1 to some vertex in V_2. Therefore, if i is a vertex in V_1 and j a vertex in V_2, there is no direct path from i to j, and thus a is not strongly connected. □

We will now prove a theorem that connects strong connectedness of the digraph of a non-negative square matrix to permutation matrices[2]. These permutation matrices will play an important role when proving that our 2^N-dimensional Hamiltonian is irreducible.

Theorem 5.6. *The graph of a square non-negative matrix a is strongly connected if and only if there exists no permutation matrix p such that*

$$p^{-1}ap = \left[\begin{array}{c|c} N & L \\ \hline 0 & R \end{array}\right]. \tag{5.2}$$

Here N and R are square matrices and 0 is the matrix with all entries zero. This holds if and only if there does not exists a non-empty proper subset $I \subset \{1,2...,n\}$ such that for all $i \in I$, and $j \in \{1,2...,n\}\backslash I$ we have $a_{ij} = 0$.

Proof. We show first that if the last assertion not holds, then necessarily there exists a permutation matrix p such that (5.2) holds.
Therefore, suppose there exists $I \subset \{1,2...,n\}$ such that $a_{ij} = 0$ if $i \in I$ and $j \in \{1,2...,n\}\backslash I$.
Let $I = \{i_{k+1},...,i_n\}$ and $I^c = \{i_1,...,i_k\}$. Define $\sigma : \{1,2...,n\} \to \{1,2...,n\}$ by $\sigma(m) = i_m \forall m \in \{1,2...,n\}$. Then σ is a permutation and for $i = k+1,..,n$ and $j = 1,...,k$, we have

$$(p_\sigma^{-1} a p_\sigma)_{ij} = a_{\sigma(i)\sigma(j)} = a_{i_i i_j} = 0. \tag{5.3}$$

Hence $(p_\sigma^{-1}ap_\sigma)$ takes the form $\left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline 0 & A_{22} \end{array}\right]$, where A_11 and A_{22} are a square matrices of dimension k and $n-k$ respectively.

Now we prove other direction, again by contraposition. Suppose there is a permutation matrix p_σ such that

$$(p_\sigma^{-1}ap_\sigma) = \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline 0 & A_{22} \end{array}\right], \tag{5.4}$$

where A_{11} and A_{22} are square matrices, for some $1 \leqslant k \leqslant n$. Then for $i = k+1,...,n$ and $j = 1,...k$, we have $(p_\sigma^{-1}ap_\sigma)_{ij} = a_{\sigma(i)\sigma(j)} = 0$. Let $I = \{\sigma(k+1),..,\sigma(n)\}$. Then the complement of I, denoted by I^c, is the set $I^c = \{\sigma(1),...,\sigma(k)\}$. Clearly, by construction $a_{II^c} = 0$.

[2]Again, these facts are take from **www.transo.com.tw/shwu/note/AMN_07.ppt**.

The next step is to show that the graph $G(a)$ is strongly connected if and only if the last statement in the proposition holds.
Suppose $G(a)$ is not strongly connected. Then $G(a)$ has at least 2 strongly connected components. So there is a $I \subset \{1, ..., n\}$ such that $(i, j) \notin E$ for all $i \in I$ and $j \in I^c$. This means that $a_{ij} = 0$ for all $i \in I$ and $j \in I^c$. Thus the last assertion does not hold.
For the other direction, suppose there is a a proper subset $I \subset \{1, ..., n\}$ such that $a_{II^c} = 0$. Then it is obvious that there is no path in $G(a)$ form vertex i to vertex j for all $i \in I$ and $j \in I^c$. Thus the graph $G(a)$ is not strongly connected. □

Now, we come to the Perron-Frobenius Theorem. It turns out that there are two versions of this theorem: one for *strictly positive* matrices, and the other for *irreducible* matrices. We will use the version for irreducible matrices since, as we shall see, the Curie-Weiss Hamiltonian -h_N^{CW} represented with respect to the standard base for $\bigotimes_{n=1}^{N} \mathbb{C}^2$ is a non-negative and irreducible matrix of dimension 2^N.

Theorem 5.7. *Let a be an $N \times N$ real-valued non-negative matrix, and denote its spectral radius by $r(a) = \lambda$. If a is irreducible, then $\lambda = r(a)$ an eigenvalue of a, which is positive, simple, and corresponds to a strictly positive eigenvector.*

In fact, the theorem also provides more results, but for us the statement above is enough. Note that this theorem is based on properties of a matrix. In fact, given some operator on a finite dimensional space, when specifying a basis and representing the operator with respect to that basis, the result will be a matrix. The matrix obtained is of course strongly dependent of the choice of the basis. Nonetheless, the Perron-Frobenius Theorem is valid if there exists a basis such that the matrix representation of the operator in this basis satisfies the assumptions of the theorem.
As we have said above, later in this chapter we will prove that our Curie-Weiss Hamiltonian -h_N^{CW}, written with respect to the canonical basis for the N-fold tensor product, is a 2^N-dimensional matrix that is non-negative and irreducible. So we could apply the above Perron-Frobenius Theorem immediately to -h_N^{CW}. When multiplying -h_N^{CW} by -1, the eigenvalues will change sign and we find instead that the smallest eigenvalue (i.e. the ground state) of h_N^{CW} is simple and corresponds to a strictly positive eigenvector. However, we will follow another approach and generalize this theorem to infinite dimensions. We will give a proof of equivalent statements of simplicity and positivity of an eigenvector based on a general setting for a σ- finite measure space. Then as a special case, we apply one of these equivalent statements to the matrix exponential $e^{-th_N^{\mathrm{CW}}}$ $(t > 0)$ in order to conclude that the ground state of h_N^{CW} is a strictly positive eigenvector, corresponding to a simple eigenvalue, and is therefore unique.

5.2 Perron-Frobenius theorem for L^2-spaces

In this section we consider a self-adjoint operator h that is bounded below and has an eigenvalue at the bottom of its spectrum. In particular, we will prove equivalent conditions stating that the eigenspace corresponding to this lowest eigenvector is one-dimensional and that the eigenvector is a strictly positive function, in a realization of the underlying Hilbert space as an L^2-space. We start with some definitions taken from [33].

Definition 5.8. *Let a be an operator on some Hilbert space $\mathcal{H}$. Then it is called bounded from below if there is a constant c such that*

$$\langle ax, x\rangle \geqslant c||x||^2 \quad (\textit{for all } x \in \mathcal{H}) \tag{5.5}$$

It follows that

$$\langle ax, x\rangle \geqslant c||x||^2 \iff \langle x, (a-c1)x\rangle \geqslant 0 \quad (\text{for all } x \in \mathcal{H}), \tag{5.6}$$

which implies that $H - c1 \geqslant 0$, so that $H \geqslant c1$ in the sense of operator ordering.

Definition 5.9. *Let $(X, d\mu)$ be a σ-finite measure space. A function $\psi \in L^2(X, d\mu)$ is called positive if ψ is non-negative almost everywhere and is not the zero function. ψ is called strictly positive if $\psi(x) > 0$ almost everywhere. A bounded operator a on L^2 is called positivity preserving if $a\psi$ is positive whenever ψ is positive. The operator a is called positivity improving if $a\psi$ is strictly positive whenever ψ is positive. Finally, a is called ergodic if and only if it is positively preserving and for any $\psi, \phi \in L^2$ that are both positive, there is some natural number $n > 0$ such that $\langle \phi, a^n\psi\rangle \neq 0$.*

Remark.
We remark that by definition the zero function is not positive. So if a is positivity preserving, then $a\psi$ is not the zero function for any positive function ψ. Moreover, every positivity improving function is ergodic: A function $\psi \in L^2(X, d\mu)$ is strictly positive if and only if $\langle \phi, \psi\rangle > 0$ for all positive functions ϕ. Thus, a bounded operator a on $L^2(X, d\mu)$ is positivity improving if and only if $\langle \phi, a\psi\rangle > 0$ for all positive functions $\phi, \psi \in L^2(X, d\mu)$. This brings us to the first theorem of this section, also stated in [33, p.204]:

Theorem 5.10. *Let h be a self-adjoint operator that is bounded from below. Let $\epsilon = inf\ \sigma(h)$. Then e^{-th} is positivity preserving for all $t > 0$ if and only if $(h-\lambda)^{-1}$ is positivity preserving for all $\lambda < \epsilon$.*

Proof. First note that e^{-th} and $(H-\lambda)^{-1}$ are bounded operators whenever $\lambda \notin \sigma(h)$. We use the following formulas

$$(h-\lambda)^{-1}\psi = \int_0^\infty e^{\lambda t}e^{-ht}\psi dt \quad (\psi \in D(h)) \tag{5.7}$$

and

$$e^{-th}\psi = \lim_{n\to\infty}\left(1 + \frac{th}{n}\right)^{-n}\psi \quad (\psi \in L^2(X, d\mu)) \tag{5.8}$$

These formulas can be proven using the theory of semigroups, or, as h is required to be self-adjoint, by functional calculus.

We can rewrite the above equation (5.8) as

$$e^{-th}\psi = \lim_{n\to\infty}\left(\frac{n}{t}(h-\tilde{\lambda})^{-1}\right)^n\psi, \tag{5.9}$$

where $\tilde{\lambda} = -\frac{n}{t}$. So if $(h-\lambda)^{-1}$ is positivity preserving for all $\lambda < \epsilon$, then for any $t > 0$ and n large enough, clearly we have $\tilde{\lambda} = -\frac{n}{t} < \epsilon$, so that also for all $t > 0$ and large n the expression $\left(\frac{n}{t}(h-\tilde{\lambda})^{-1}\right)^n$ is positivity preserving, hence e^{-th} is positivity preserving.

On the other hand, if e^{-th} is positivity preserving for all $t > 0$, then from (5.7), it follows that $(h-\lambda)^{-1}$ is positivity preserving. □

The above theorem will be used in order to prove the main theorem (Theorem 5.11 below), which proves positivity of the ground state. This theorem is a combination of [33, Thm. XIII.43] and [33, Thm. XIII.44].

Theorem 5.11. *Let h be a self-adjoint operator on $L^2(X, d\mu)$ that is bounded from below. Suppose e^{-th} is positivity preserving for all $t > 0$ and that $\epsilon = inf\ \sigma(h)$ is an eigenvalue of h. Then the following are equivalent:*

(a) ϵ is a simple eigenvalue of h with a strictly positive eigenvector.
(b) e^{-th} is ergodic for some $t > 0$.
(c) $L^\infty(X) \cup \{e^{-th}\}$ acts irreducibly for some $t > 0$, i.e., no non trivial closed subspace is left invariant by both e^{-th} and every bounded multiplication operator.
(d) $(h - \lambda)^{-1}$ is ergodic for some $\lambda < \epsilon$.
(e) $(h - \lambda)^{-1}$ is positivity improving for all $\lambda < \epsilon$.
(f) e^{-th} is positivity improving for all $t > 0$.

Before we proof all equivalent statements, we say something about the application of this theorem to the Curie-Weiss Hamiltonian (3.1) and the quantum mechanical double well Hamiltonian as given by (4.93) in the previous chapter. In the next paragraph we are going to prove that the Curie-Weiss Hamiltonian $-h_N^{\mathrm{CW}}$, represented with respect to the canonical basis for $\bigotimes_{n=1}^N \mathbb{C}^2$, has a strictly positive matrix exponential for all $t > 0$, and that h_N^{CW} satisfies the assumptions of Theorem (5.11). Then we can indeed apply the equivalence between statements (a) and (f) from this theorem to our Curie-Weiss matrix in order to conclude that this Hamiltonian has a unique strictly positive eigenvector corresponding to the simple eigenvalue ϵ. In fact, it is enough to prove the equivalence $(a) \iff (f)$, rather then all other other statements. But in the literature, this equivalence is not directly proven and is often based on other lemmas. In this thesis, all these lemmas are added in one single theorem in order to compare the equivalent statements easily.
Moreover, this theorem shows also that the Perron-Frobenius Theorem in the linear algebra setting (Theorem (5.7)) follows as a special case of this more general theorem, which holds for a much bigger class of operators than only the non-negative irreducible matrices.
Furthermore, in §5.4 we will see how the uniqueness of the ground state of the (unbounded) quantum mechanical double well Hamiltonian can be proved using this theorem.

Proof. $(a) \implies (b)$.
Since ϵ is a simple eigenvalue of h, it follows that $e^{-t\epsilon}$ is a simple eigenvalue of e^{-th} for all $t > 0$. Clearly, $e^{-t\epsilon}$ is the largest eigenvalue corresponding to e^{-th}. Put $b = e^{-th}/||e^{-th}||$. Then, by functional calculus, b is positive and we have $b \leqslant ||b|| = 1$. Let $\{P_\Omega\}$ be the spectral projections for b. Consider the map $f_n(x) = x^n$ on $[0, 1]$. Then $f_n \to \chi_1$ pointwise, with χ_1 the characteristic function in 1. By the measurable functional calculus applied to the self-adjoint element b, we have

$$f_n(b) \mapsto f(b) \quad \text{strongly.} \tag{5.10}$$

But $f(b) = \chi_1(b)$ is just the spectral projection $p_{\{1\}}$ for b. This is the projection onto the kernel of $b - 1I$, i.e the eigenspace for 1. By assumption, $1 = ||b||$ is a simple eigenvalue for b. It follows by hypothesis that $p_{\{1\}} = \langle\psi, \cdot\rangle\psi$ for some strictly positive ψ. Then for any positive χ and ϕ, we have

$$\lim_{n\to\infty} \langle\phi, b^n\chi\rangle = \langle\phi, \psi\rangle\langle\psi, \chi\rangle > 0, \tag{5.11}$$

where we used the fact that strong convergence implies weak convergence. Hence there exists a natural number n such that $\langle\phi, (e^{-th})^n\chi\rangle = ||e^{-th}||^n\langle\phi, b^n\chi\rangle > 0$. Thus e^{-th} is ergodic.

$(b) \implies (c)$.
Suppose by contraposition that c does not hold. Then we can find a non-trivial left-invariant subspace S for $L^\infty(X) \cup \{e^{-th}\}$. Let $f \in S$ and put $h = \bar{f}/|f| \in L^\infty(X)$. Then $|f| = |f|^2/|f| = hf \in S$. Similarly, for $g \in S^\perp$, it follows that $|g| \in S^\perp$. Now, pick $f \in S$,

and $g \in S^\perp$ such that $f, g \neq 0$. Since e^{-th} leaves S invariant, we have that $e^{-nth}|f| \in S$ for all n, hence

$$\langle |g|, e^{-nth}|f| \rangle = 0 \tag{5.12}$$

for all n. Thus e^{-th} is not ergodic.

$(c) \implies (a)$.
By hypothesis, ϵ is an eigenvalue. Let ψ be the eigenvector of e^{-th} corresponding to $e^{-t\epsilon}$. Suppose first that ψ is real-valued. Then as $|\psi| \pm \psi \geqslant 0$, we know that $e^{-th}(|\psi| \pm \psi) \geqslant 0$, since e^{-th} is positivity preserving. Hence

$$0 \leqslant |e^{-th}\psi| \leqslant e^{-th}|\psi|. \tag{5.13}$$

It follows that

$$e^{-t\epsilon}||\psi||^2 \geqslant \langle |\psi|, e^{-th}|\psi| \rangle \geqslant \langle |\psi|, |e^{-th}\psi| \rangle \geqslant \langle \psi, e^{-th}\psi \rangle = e^{-t\epsilon}||\psi||^2. \tag{5.14}$$

In the first step, we used Cauchy-Schwarz and the fact that $e^{-t\epsilon}$ is the largest eigenvalue of the self-adjoint operator e^{-th}, which equals its spectral radius, just being this eigenvalue. In the second and third steps, we used the positivity preserving property of e^{-th} applied to the positive function $e^{-th}|\psi| - |e^{-th}\psi|$ and to $|e^{-th}\psi| - e^{-th}\psi$. In the last step we used $e^{-th}\psi = e^{-t\epsilon}\psi$. So all the inequalities become equalities.

Now, if $|e^{-th}\psi| < e^{-th}|\psi|$, then $e^{-th}|\psi| - |e^{-th}\psi| > 0$, so that it follows that $\langle |\psi|, e^{-th}|\psi| \rangle > \langle |\psi|, |e^{-th}\psi|$, which is a contradiction by the above. As a result, $e^{-th}|\psi| = e^{-\epsilon t}|\psi|$, so $|\psi|$ is also an eigenvector. We show that $|\psi|$ is strictly positive.

Let $S = \{f \in L^2(X, d\mu) |\ f\psi = 0 \ a.e.\}$. Then S is clearly a closed subspace and is left invariant by $L^\infty(X)$. Let $S_+ = \{g \in S |\ g \geqslant 0\}$. Then for $f \in S_+$,

$$\langle e^{-th}f, |\psi| \rangle = \langle f, e^{-th}|\psi| \rangle = e^{-t\epsilon}\langle f, |\psi| \rangle = 0. \tag{5.15}$$

The last step in the above equality follows from the observation:

$$\langle f, |\psi| \rangle = \int_X \overline{f}|\psi| = \int_X |f||\psi| = \int_X |f\psi| = 0, \tag{5.16}$$

where the first equality follows by definition of the inner product, the second by positivity of f, and the last equality from the fact that $f \in S_+$. Then it follows that

$$\int_X (e^{-th}f)|\psi| = \langle e^{-th}f, |\psi| \rangle = \|e^{-t\epsilon}\| \langle f, |\psi| \rangle = 0, \tag{5.17}$$

where used in the first step that $e^{-th}f$ is positive.
Since also $|\psi|$ is positive, the product $(e^{-th}f)|\psi|$ is positive, and since the integral of this function is zero, it follows that $(e^{-th}f)|\psi| = 0$ almost everywhere. Furthermore, for any $f \in L^2(X)$ any $x \in X$, $(f\psi)(x) = 0$ if and only if $(f|\psi|)(x) = 0$. So, $((e^{-th}f)|\psi|)(x) = 0$ if and only if $((e^{-th}f)\psi)(x) = 0$. We conclude that $e^{-th}f \in S_+$, thus e^{-th} leaves S_+ invariant. Since

$$S = S_+ - S_+ + i(S_+ - S_+), \tag{5.18}$$

e^{-th} leaves S invariant. By hypothesis (c), $S = \{0\}$ or $S = L^2(X)$. But since $\psi \notin S$,and $\psi \neq 0$ (because it is an eigenvector), it follows that $S = \{0\}$. Then $|\psi| > 0$ a.e.

Thus any real eigenvector with eigenvalue $e^{-t\epsilon}$ is nonzero a.e., and satisfies $e^{-th}|\psi| = \|e^{-t\epsilon}\||\psi|$. Thus $|\psi| - \psi$ is an eigenvector with eigenvalue $e^{-t\epsilon}$, or it is identically zero, so that $|\psi| - \psi$ is either almost everywhere vanishing or almost everywhere nonvanishing. This means that every real eignvector with eigenvalue $e^{-t\epsilon}$ is almost everywhere strictly positive (in the case that $|\psi| - \psi = 0$ a.e) or almost everywhere strictly negative (in the case that $|\psi| - \psi \neq 0$ a .e.)
If e^{-th} had two real different eigenvectors with eigenvalue $e^{-t\epsilon}$, we can assume that they are linearly independent (because eigenvectors are unique up to scalar multiplication). Then the operator would also have two orthogonal eigenvectors, which follows from the Gram-Schmidt process for the eigenspace. Both eigenvectors can be chosen positive a.e, since if for example one of the real eigenvectors is strictly negative a.e, then multiplying it by -1 gives an a.e. strictly positive eigenvector. But this is impossible by definition of the L^2-inner product. We conclude that e^{-th} has only one real eigenvector of eigenvalue $e^{-t\epsilon}$ and this eigenvector is strictly positive a.e.
Finally, let ψ be an arbitrary eigenvector with eigenvalue $e^{-t\epsilon}$. Since e^{-th} is a positive operator, it maps positive functions into positive functions, so by linearity it takes real functions into real functions. Thus $A(\mathrm{Re}(\psi)) = \mathrm{Re}(A\psi)$. Since $\psi(x) = \mathrm{Re}(\psi)(x) + i \cdot \mathrm{Im}(\psi)(x)$, where $\mathrm{Re}(\psi)$ and $\mathrm{Im}(\psi)$ are both real, it follows that both $\mathrm{Re}(\psi)$ and $\mathrm{Im}(\psi)$ are real eigenvectors with eigenvalue $e^{-t\epsilon}$. We conclude that ψ is a complex multiple of the unique real (strictly positive) eigenvector. Hence $e^{-t\epsilon}$ is a simple eigenvalue corresponding to a strictly positive eigenvector.

$(b) \implies (d)$.
From the proof of Theorem 5.10, we can write

$$(h-\lambda)^{-1} = \int_0^\infty e^{\lambda t} e^{-ht} dt \quad (\lambda < \epsilon). \tag{5.19}$$

We must show for a fixed $\lambda < \epsilon$, that for all positive functions $f, g \in L^2$, we have $\langle f, (h-\lambda)^{-n} g\rangle \neq 0$ for some $n > 0$ and that $(h-\lambda)^{-1}$ is positively preserving. We start with the last assertion. Suppose e^{-th} is ergodic from some $t > 0$. Since, by assumption, e^{-th} is positively preserving for all $t > 0$, it follows by Theorem 5.10 that $(h-\lambda)^{-1}$ is positively preserving for all $\lambda < \epsilon$.

Now we prove the ergodic property for $(h-\lambda)^{-1}$. By assumption, e^{-th} is ergodic for some $t > 0$. So for all positive functions f, g, there is an $n > 0$ such that $\langle f, e^{-nth} g\rangle > 0$. Put $s = nt > 0$. Notice that $\langle f, e^{-sh} g\rangle$ is continuous, so $\langle f, e^{-sh} g\rangle > 0$ on some interval containing s. Thus for any $\lambda < \epsilon$

$$\langle f, (h-\lambda)^{-1} g\rangle = \int_0^\infty e^{\lambda x} \langle f, e^{-hx} g\rangle dx > 0. \tag{5.20}$$

Now, for this n we compute

$$\langle f, (h-\lambda)^{-n} g\rangle = \langle (h-\lambda)^{-n+1} f, (h-\lambda)^{-1} g\rangle = \int_0^\infty e^{\lambda x} \langle (h-\lambda)^{-n+1} f, e^{-xh} g\rangle dx. \tag{5.21}$$

This integral is strictly positive if $\langle (h-\lambda)^{-n+1} f, e^{-th} g\rangle$ is strictly positive on some interval. By the above, for all positive functions f, g, the expression $\langle f, e^{-sh} g\rangle > 0$ on an interval containing s, so we are done if we show that $(h-\lambda)^{-n+1} f$ is positive, since in this case, there would exists an $\tilde{n}$ such that $\langle (h-\lambda)^{-n+1} f, e^{-\tilde{n}th} g\rangle > 0$, which by continuity holds also on an interval.

So we need to show that $(h-\lambda)^{-n+1}$ is positively preserving. But

$$\langle f,(h-\lambda)^{-n+1}g\rangle = \langle f,(h-\lambda)^{-n+2}(h-\lambda)^{-1}g\rangle = \int_0^\infty e^{\lambda x}\langle (h-\lambda)^{-n+2}f, e^{-xh}g\rangle dx. \tag{5.22}$$

By the same argument as above, we show that $(h-\lambda)^{-n+2}$ is positivity preserving. This process can be repeated $n-2$ times, so that it follows that we just have to prove that $(h-\lambda)^{-1}$ is positivity preserving. But this statement was already proven by (5.20). Hence $(h-\lambda)^{-n+1}$ is positivity preserving. We conclude that $\langle f,(h-\lambda)^{-n}g\rangle > 0$. Thus $(h-\lambda)^{-1}$ is ergodic.

$(d) \implies (b)$.
Assume $(h-\lambda)^{-1}$ is ergodic for some $\lambda < \epsilon$. We need to show that there is a $t>0$ such that for all positive f,g there is some $n>0$ such that $\langle f, e^{-tnh}g\rangle \neq 0$. By assumption, e^{-th} is positivity preserving for all $t>0$. So $\langle f, e^{-th}g\rangle \geqslant 0$ for all $t>0$. As before, compute

$$0 \neq \langle f,(h-\lambda)^{-n}g\rangle = \int_0^\infty e^{\lambda x}\langle (h-\lambda)^{-n+1}f, e^{-xh}g\rangle dx. \tag{5.23}$$

This inner product in the integrand is equal to

$$\begin{aligned}\langle (h-\lambda)^{-n+1}f, e^{-xh}g\rangle &= \langle (h-\lambda)^{-n+2}f, (h-\lambda)^{-1}(e^{-xh}g)\rangle = \\ &\int_0^\infty e^{\lambda y}\langle (h-\lambda)^{-n+2}f, e^{-yh}e^{-xh}g\rangle dx = \\ &\int_0^\infty e^{\lambda y}\langle (h-\lambda)^{-n+2}f, e^{-(x+y)h}g\rangle dx.\end{aligned} \tag{5.24}$$

Iterating this process, we find that

$$0 \neq \langle f,(h-\lambda)^{-n}g\rangle = \int_0^\infty \cdots \int_0^\infty e^{\lambda(x_1+\ldots+x_n)}\langle f, e^{-(x_1+\ldots+x_n)h}g\rangle dx_1\cdots dx_n. \tag{5.25}$$

If for all $t>0$ the expression $\langle f, e^{-th}g\rangle$ equals 0, then also the above integral is zero and we have a contradiction. So there is a $t>0$ such that $\langle f, e^{-th}g\rangle > 0$, and by continuity, this inequality holds on an interval so that the integral is strictly positive. Then take $n=1$, and we have shown that e^{-th} is ergodic.

$(d) \implies (e)$
Let f and g be positive. Since e^{-th} is ergodic, $\langle f, e^{-sh}g\rangle > 0$ for some > 0. But $s \mapsto \langle f, e^{-sh}g\rangle$ is continuous in s, so $\langle f, e^{-sh}g\rangle > 0$ on some interval containing s. Thus for all $\lambda < \epsilon$,

$$\langle f,(h-\lambda)^{-1}g\rangle = \int_0^\infty e^{\lambda s}(\langle f, e^{-sh}g\rangle ds > 0. \tag{5.26}$$

$(d) \implies (f)$
Let f and g be positive and put $B = \{t>0 \mid \langle f, e^{-th}g\rangle > 0\}$.
The map $t \mapsto (f, e^{-tH}g)$ is analytic on $(0,\infty)$, which means that every zero of this map is an isolated point. But $(0,\infty)\backslash B$ is precisely the set of zeros of this map in $(0,\infty)$. So for any $x \in (0,\infty)$ there exists an $\varepsilon > 0$ such that for any $y \in (0,\infty)\backslash B$, $y \neq x$, we have $|x-y| \geqslant \varepsilon$.

If x would be a limit point of $(0,\infty)\backslash B$, then for any $\varepsilon > 0$ there exists a $y \in (0,\infty)\backslash B$,

such that $|x-y| < \varepsilon$. Such a point x has to be in the closure of $(0,\infty)\backslash B$, but by definition, it cannot be in $(0,\infty)\backslash B$ itself. Since every isolated point is not a limit point and every limit point is not an isolated point, by the previous observation, it now follows that the closure of $(0,\infty)\backslash B$ is a subset of $[0,\infty)\backslash B$. Hence $x \in ([0,\infty)\backslash B)\backslash((0,\infty)\backslash B) \subseteq \{0\}$. The conclusion is that if $(0,\infty)\backslash B$ has a limit point, it is equal to one. In particular, B contains arbitrary small numbers. Thus, if we can show that $t > s$ and $s \in B$ implies that $t \in B$, we can conclude that $b = (0,\infty)$.
Fix $s \in B$. Then $(f, e^{-th}g) > 0$, so that $f(\cdot)(e^{-th}g)(\cdot)$ is not identically zero. Put $w = \min(f, e^{-sh}g)$. Then w is not identically zero since f is positive and also $e^{-sh}g$ is not identically zero because e^{-sh} is positively preserving and g positive. It follows that for any $\tau > 0$,

$$\begin{aligned}\langle f, e^{-\tau h}(e^{-sh}g)\rangle &\geqslant \langle f, e^{-\tau h}w\rangle = \langle e^{-\tau h}f, w\rangle \\ &\geqslant \langle e^{-\tau h}w, w\rangle = \|e^{-\tau h/2}w\|^2 > 0. \end{aligned} \tag{5.27}$$

We have used that w is positive and that $e^{-\tau h/2}$ is positively preserving to conclude that $e^{-\tau h/2}w \neq 0$. Thus $s \in B$ and $\tau > 0$ imply that $s + \tau \in B$.

$(e) \implies (d)$
This follows from the remark before Theorem 5.10.

$(f) \implies (b)$
Again, this follows by the same remark. □

5.3 Perron-Frobenius theorem and the Curie-Weiss model

The general theorem from the previous paragraph can of course also be applied to (some class) of matrices, by taking X as a discrete space with counting measure. We will prove that the matrix exponential $e^{-th_N^{\mathrm{CW}}}$ of the Curie-Weiss Hamiltonian $-h_N^{\mathrm{CW}}$ is positivity improving for all $t > 0$. For this, we need a lemma that connects irreducibility of a non-negative square matrix to its matrix exponential. The proof of this lemma is based on [11].

Lemma 5.12. *If a is non-negative matrix, then it is irreducible if and only if the matrix exponential e^a is strictly positive in the sense of Definition* 5.1.

Proof. Take $\alpha \in \mathbb{R}_+$ such that $1/\alpha$ is greater than the spectral radius of a. Then we know that $(1-\alpha a)^{-1} =: S$ exists, and S is given by the Neumann series

$$S = 1 + \alpha a + \alpha^2 a^2 + \alpha^3 a^3 + ... \tag{5.28}$$

This follows since this sum of the Neumann series on he right hand side exists and it is easy to see that $(1-\alpha a)S = 1 = S(1-\alpha a)$. Now, for any $i, j \in \mathbb{R}$, the matrix entry $S_{i,j}$ is a sum of non-negative terms and if S is strictly positive, then there must be a lowest power $m_{i,j}$ of S such that $a^{m_{i,j}} > 0$, since the identity matrix is not strictly positive. By the previous definition, if this is true for all i, j, then a is irreducible.
Conversely, if a is irreducible, then for all indices i and j, there must be a power m of a such that $(a^m)_{ij} > 0$. This implies that for all i and j there must be terms in $S_{i,j}$ that are non-zero.
Now, we apply this to e^a. This matrix exponential is defined by the power series

$$e^a = 1 + a + \frac{a^2}{2!} + \frac{a^3}{3!} + ... \tag{5.29}$$

The above argument applies for $S = e^a$. Hence a is irreducible if and only if e^a is strictly positive. □

Now, we are in a position to prove a statement about our Hamiltonian $-h_N^{CW}$. This statement will depend on the basis in which we represent the operator. We will take the standard basis of $\mathbb{C}^2$, also extended to a basis of the tensor product $\bigotimes_{n=1}^N \mathbb{C}^2$.

Theorem 5.13. *The Curie-Weiss Hamiltonian $-h_N^{CW}$ from (3.1), represented in the standard basis for $\bigotimes_{n=1}^N \mathbb{C}^2$, is non-negative and irreducible.*

Proof. Since all constant factors in $-h_N^{CW}$ are strictly positive, we only have to consider both terms containing sums. We show that

$$\sum_{x,y\in\Lambda_N} \sigma_3(x)\sigma_3(y) + \sum_{x\in\Lambda_N} \sigma_1(x) \tag{5.30}$$

is non-negative. Consider the standard basis $\{e_1, e_2\}$ for $\mathbb{C}^2$ over $\mathbb{C}$. Then $\{e_{n_1}\otimes ...\otimes e_{n_N}\}_{n_1=1,...,n_N=1}^2$ is the standard basis for $\bigotimes_{n=1}^N \mathbb{C}^2$. Note that the spin-Pauli matrix σ_3 maps e_1 to e_1 and e_2 to $-e_2$, whereas σ_1 maps e_1 to e_2 and e_2 to e_1. Note that $\sigma_1(x) = 1\otimes ...\otimes 1\otimes\sigma_1\otimes 1...\otimes 1$, where σ_1 acts on the x^{th} position and similarly for $\sigma_3(x)$. It follows for all $x, y \in \{1, ..., N\}$ that

$$\begin{aligned}
&\sigma_3(x)(e_{n_1}\otimes ...\otimes e_{n_N}) = \\
&1(e_{n_1})\otimes ...\otimes 1(e_{n_{x-1}})\otimes\sigma_3(e_{n_x})\otimes 1(e_{n_{x+1}})\otimes ...\otimes 1(e_{n_N}) = \\
&\begin{cases} +e_{n_1}\otimes ...\otimes e_{n_N}), \text{ if } e_{n_x} = \begin{pmatrix}1\\0\end{pmatrix} \\ -e_{n_1}\otimes ...\otimes e_{n_N}), \text{ if } e_{n_x} = \begin{pmatrix}0\\1\end{pmatrix}. \end{cases}
\end{aligned} \tag{5.31}$$

We have $\sigma_3(y)\sigma_3(x)(e_{n_1}\otimes ...\otimes e_{n_N}) = \pm(e_{n_1}\otimes ...\otimes e_{n_N})$, where the minus sign appears only if $e_{n_x} \neq e_{n_y}$. We conclude that the standard basis for the N-fold tensor product is a set of eigenvectors for $\sigma_3(y)\sigma_3(x)$ with eigenvalues ± 1. Thus we know that $\sum_{x,y\in\Lambda_N}\sigma_3(x)\sigma_3(y)$ is a diagonal matrix with respect to this standard basis.

The entries are all non-negative.
This can easily be seen by the following argument. Given an arbitrary basis vector $e := (e_{n_1}\otimes ...\otimes e_{n_N})$, let A be the set of indices of this vector containing e_1, and B the set of indices containing e_2. Let $a = \#A$, and $b = \#B$, so that $a + b = n$. Then $\sigma_3(x)\sigma_3(y)e$ has a negative eigenvalue -1 if and only if $x \in A$ and $y \in B$, or $x \in B$ and $y \in A$. In the sum $\sum_{x,y\in\Lambda_N}\sigma_3(x)\sigma_3(y)e$, this gives $ab + ba = 2ab$ minus signs. So there are $n^2 - 2ab$ plus signs. We must have, independently of a and b, that $n^2 - 2ab \geqslant 2ab$, and then we are done, since the diagonal term can be never strictly negative. Plugging in $a + b = n$ gives $n^2 - 4a(n - a) \geqslant 0$ if and only if $n^2 - 4an + 4a^2 \geqslant 0$. The parabola $a \mapsto n^2 - 4an + 4a^2$ attains its minimum in $a = n/2$, which is given by $n^2 - 4\frac{n}{2}n + 4(\frac{n}{2})^2 = 0$. So indeed, there are at least as much plus signs as minus signs so that the corresponding diagonal term is non-negative.

The other term $\sum_{x\in\Lambda_N}\sigma_1(x)$ does not contain any negative entries at all, so if we apply this to any basis vector $\{e_{n_1}\otimes ...\otimes e_{n_N}\}$, we get a non-negative matrix. It follows that the (5.30) is non-negative.

Now we show that the matrix corresponding to the Curie-Weiss Hamiltonian is irreducible. Note that irreducibility of a matrix does not depend on the basis in which the operator is represented, since similar matrices define equivalent representations which preserve irreducibility.
We use Theorem 5.6 to show by contradiction that the matrix $-h_N^{CW}$ is irreducible.
So suppose there exists a permutation matrix p such that

$$p^{-1}(-h_N^{CW})p = \left[\begin{array}{c|c} N & L \\ \hline 0 & R \end{array}\right]. \tag{5.32}$$

Now $-h_N^{CW}$ is symmetric, since all σ_1 and σ_3 are symmetric. It follows that $L = 0$. Moreover,

$$x := p^{-1} \sum_{x,y \in \Lambda_N} \sigma_3(x)\sigma_3(y)p \tag{5.33}$$

is again a diagonal matrix and $y := \sum_{x \in \Lambda_N} \sigma_1(x)$ commutes with any permutation operator since it is a sum over all spin flips. It follows that the only off-diagonal terms in $p^{-1}(-h_N^{CW})p$ are coming from the part $\sum_{x \in \Lambda_N} \sigma_1(x)$. But if we take the $2^N/2$-th basis vector, i.e. $e := (e_1 \otimes e_2 \otimes ... \otimes e_2)$ in the ordered basis as defined before, then $\sigma_1(1)e = (e_2 \otimes e_2 \otimes ... \otimes e_2)$. Thus in this matrix representation, the last basis vector contributes. Hence we see that in the matrix $p^{-1}(-h_N^{CW})p$ on position $(2^N, 2^N/2)$ there is always a 1. We can repeat this process for the vector that has the vector e_2 only in two positions. So there is also a 1 at position $(2^N - 1, 2^N/2 - 1)$, and so on. In the last step we see that there is a 1 at position $(2^N/2 + 1, 1)$, It follows that the blocks N and R can never be square. This is a contradiction.

We have showed that the non-negative matrix $-h_N^{CW}$ is irreducible. Thus the Curies-Weiss Hamiltonian is a non-negative irreducible matrix. □

We are going to use Theorem 5.11 and Lemma 5.12. By the previous proposition, we may apply Lemma 5.12 to the Curie- Weiss Hamiltonian $-h_N^{CW}$. Then $e^{-h_N^{CW}}$ is strictly positive. Then clearly for any $t > 0$, also $e^{-th_N^{CW}}$ is strictly positive. Furthermore, it is positivity improving. To see this, we must show that for any to non-zero positive vectors $f, g \in L^2(X, d\mu)$, we have

$$\langle f, e^{-th_N^{CW}} \rangle_{L^2} > 0. \tag{5.34}$$

Since our space X is a discrete space consisting of 2^N points, the corresponding measure is simply the counting measure. Hence the inner product is just the standard inner product on $\mathbb{C}^{2^N}$. Moreover it suffices to show the above inequality for (standard) basis vectors e_i, where $1 \leqslant i \leqslant 2^N$, So we are done if we show that for all i and j,

$$\sum_{i=1}^{i=2^N} e_i(k)(e^{-th_N^{CW}} e_j)(k) > 0. \tag{5.35}$$

The above equation means that $(e^{-th_N^{CW}} e_j)(i) > 0$, which is saying that all entries of the matrix are strictly positive. So this means that for all $t > 0$, $e^{-th_N^{CW}}$ is positivity improving, which is exactly what we just have shown.
It remains to show that $-h_N^{CW}$ is bounded from below. But this is obvious, since any matrix is bounded from below. In order to apply Theorem (5.11), inf $\sigma(h_N^{CW})$ must be an eigenvalue. But this is trivial in a finite dimensional Hilbert space. The positivity improving Curie-Weiss Hamiltonian satisfies all the assumptions of Theorem (5.11), so that we may conclude that the lowest eigenvalue is simple, with a strictly positive eigenvector.

It also follows that Theorem 5.11 can be applied to $-a$, for any non-negative irreducible self-adjoint matrix a, since then e^{ta} $(t > 0)$ is strictly positive, and automatically every matrix is bounded from below by its spectral radius and the bottom of the spectrum is always an eigenvalue. Thus for these matrices, the eigenvalue corresponding to the ground state will be simple and the ground state eigenvector is strictly positive. Of course, Theorem 5.11 does not hold only for matrices, and can therefore be seen a generalization of this version of the Perron-Frobenius Theorem, given in Theorem 5.7.

5.4 Application to Schrödinger operators

We have seen in Chapter 3 that the scaled compressed Curie-Weiss Hamiltonian $\frac{1}{N}h_N^{\mathrm{CW}} \restriction_{\mathrm{sym}^N(\mathbb{C}^2)}$, written with respect to the canonical base for $\mathrm{sym}^N(\mathbb{C}^2)$, was a tridiagonal matrix of dimension $N+1$. In Chapter 4, we have argued that this scaled matrix was related to an unbounded Schrodinger operator describing a particle in a symmetric double well potential. Therefore, we will also explain how the Perron-Frobenius Theorem for matrices can be generalized to some class of unbounded operators on an infinite Hilbert space. In this section we prove a general theorem stating that the Schrodinger operator with a locally integrable potential V bounded from below such that $\lim_{|x|\to\infty} V(x) = \infty$, has has a non-degenerate strictly positive ground state. The proof of this statement is partially based on Theorem (5.11) and on other theorems that we will prove in this chapter. In particular, the harmonic oscillator with a symmetric double well potential one the real line will be an example. However, we will prove the theorem for the Hilbert space $L^2(\mathbb{R}^n)$, with n an arbitrary natural number. It is not so easy to prove this statement for arbitrary n. Therefore, in Appendix D we give some important definitions and basis facts about unbounded operators.
Using the machinery from this appendix, we can start with the theorems regarding the Schrodinger operator with some class of potentials. We consider potentials that are bounded from below and such that $\lim_{|x|\to\infty} V(x) = \infty$. The main theorem of this section is:

Theorem 5.14. *Let $V \in L^2_{loc}(\mathbb{R}^n)$ be positive and suppose that $\lim_{|x|\to\infty} V(x) = \infty$. Then $-\overline{\Delta + V}$ has a non-degenerate strictly positive ground state.*

The notation $-\overline{\Delta + V}$ is explained by (D.4). It denotes the closure of the operator $\Delta + V$. The above theorem can be found in [33, Thm. XIII.47]. However, the proof is quite short. We try to give a more detailed version of it. The proof we provide basically consists of three steps. The first step we is to show that the spectrum of the operator $H = \overline{-\Delta + V}$ is discrete. We need a couple of theorems in order to prove this. The first theorem involved is based of the compactness of the resolvent operator:

Theorem 5.15. *Let $V \in L^1_{loc}(\mathbb{R}^n)$ be bounded from below and suppose that $V(x) \to \infty$ if $|x| \to \infty$. Then $H = -\Delta + V$, defined as a sum of quadratic forms, is an operator with compact resolvent.*

This statement can be proven using the min-max principle, as given in [33, Thm. XIII.1]. However, we give a more direct proof based on the following theorem:

Theorem 5.16. *Let $V \in L^1_{loc}(\mathbb{R}^n)$ be bounded from below and suppose that $V(x) \to \infty$ if $|x| \to \infty$. Then the injection of $H^1_V(\mathbb{R}^n)$ into $L^2(\mathbb{R}^n)$ is compact.*

To prove this theorem, we need the following two lemmas and a corollary. These can be found in [7, section 4.1]. The proofs involve Sobolev spaces H^s with a real parameter s. More information about these spaces can be found in Appendix D or in [9].

Lemma 5.17. *Let V be a real measurable function on $\mathbb{R}^n$ such that:*
(a) $V(x)$ tends to 0 if $x \to \infty$;
(b) multiplication by V is a continuous mapping from $H^s(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$, for a particular $s \geqslant 1$.

Then multiplication by V is a compact mapping from $H^t(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$, for all $t > s$.

Proof. Let $\varphi \in \mathcal{D}(\mathbb{R}^n)$ be a test function with $\varphi = 1$ for $|x| < 1$, and $\varphi_k(x) = \varphi(x/k)$ with $k \in \mathbb{N}$. Let T_k be the mapping from $H^s(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$ defined by:

$$T_k u(x) = \varphi_k(x)V(x)u(x) \quad (x \in \mathbb{R}^n), \tag{5.36}$$

being the composition of the mapping: $u \in H^t(\mathbb{R}^n) \mapsto \varphi_k u \in H^s(\mathbb{R}^n)$ and multiplication by V. It is a general fact that $u \in H^t(\mathbb{R}^n) \mapsto \varphi_k u \in H^s(\mathbb{R}^n)$ is compact and, by assumption, multiplication by V is continuous, so that T_k is therefore compact. Furthermore, for all $u \in H^t(\mathbb{R}^n)$

$$||T_k u - Vu|| = ||(1-\varphi_k)Vu|| = \left(\int_{|x|>k} |(1-\varphi_k)Vu|^2 dx \right)^{1/2} \tag{5.37}$$

$$\leqslant A \sup_{|x|>k} |V(x)| ||u||_{L^2}^{1/2} \leqslant A \sup_{|x|>k} |V(x)| ||u||_{H^1}. \tag{5.38}$$

Here, A is a constant given by the supremum of $|1-\varphi_k|$ times the length of the (compact) interval where $\varphi_k \neq 0$. When $k \to \infty$, for all $|x| > k$ we clearly have $\varphi_k \to 0$, as it is a test function. Since $t > s$ we know that $H^t \subset H^s \subset H^1$ so that $||u||_{H^1}$ is finite, since its norm can be bounded by $||u||_{H^t}$. Now, by taking $k \to \infty$, we see that the sequence of compact operators T_k converges, for the norm topology in $B(H^t(\mathbb{R}^2), L^2(\mathbb{R}^2))$, towards the operator of multiplication by V, which is therefore compact. □

Lemma 5.18. *Let p be a real measurable function on $\mathbb{R}^n$ such that:*
(a) $1/p \in L^2_{loc}(\mathbb{R}^n)$;
(b) multiplication by p is a compact mapping from $H^s(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$, for some $s > 0$.

Then the space V defined by:

$$V = \{u \in H^s(\mathbb{R}^n) : \int \frac{|u(x)|^2}{|p(x)|^2} dx < \infty\}, \tag{5.39}$$

equipped with the norm:

$$||u||_V = \left(||u||_{H^s}^2 + \int \frac{|u(x)|^2}{|p(x)|^2} dx \right)^{1/2} \tag{5.40}$$

is contained in $L^2(\mathbb{R}^n)$ with compact injection.

Proof. We have to show that the inclusion operator $\iota : H^s(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is compact in that the image $(\iota(u_k))_k$ of any weakly convergent sequence $(u_k)_k \in V$ converges in L^2- norm. Therefore, given such a weakly convergent sequence $(u_k)_k$ in V, without loss of generality we may assume that $(u_k)_k$ is bounded by one and that it converges to 0. Thus, we have the following setting: $(u_k)_k$ is a sequence of elements $u_k \in V$ such that

$$||u_k||_V \leqslant 1, \quad u_k \to 0 \ \text{ in } \ V \ \text{ weakly if } \ k \to \infty. \tag{5.41}$$

Since $||u_k||_H^s \leqslant ||u_k||_V$, the space V is contained in the space $H^s(\mathbb{R}^n)$, with continuous injection, we deduce that the sequence $(u_k)_k$ satisfies

$$||u_k||_{H^s} \leqslant 1, \quad u_k \to 0 \ \text{ in } \ H^s(\mathbb{R}^n) \ \text{ weakly if } \ k \to \infty. \tag{5.42}$$

From the compactness of multiplication by $p : H^s(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, we have

$$||pu_k||_{L^2} \to 0 \ \text{ if } \ k \to \infty. \tag{5.43}$$

By hypothesis: $||u_k||_V \leqslant 1$ implies that $\int \frac{|u_k|^2}{|p|^2} dx \leqslant 1$, whence by Cauchy-Schwarz inequality:

$$\int |u_k|^2 dx = \int p u_k \frac{u_k}{p} dx \leqslant \left(\int |pu_k|^2 dx \right)^{1/2} \left(\int |\frac{u_k}{p}|^2 dx \right)^{1/2}, \tag{5.44}$$

hence

$$||u_k||_{L^2}^2 \leqslant ||pu_k||_{L^2}, \tag{5.45}$$

which shows that $||u_k||_{L^2} \to 0$ if $k \to \infty$. This proves the lemma. □

This brings us to the following corollary.

Corollary 5.19. *Let $V \in L^1_{loc}(\mathbb{R}^n)$ be bounded from below and suppose that $V(x) \to \infty$ if $|x| \to \infty$. For all given $\alpha > 0$, the space $W \equiv W_\alpha$ defined by,*

$$W = \{y \in H^1(\mathbb{R}^n) : \ (1+V)^\alpha u \in L^2(\mathbb{R}^n)\}, \tag{5.46}$$

with norm

$$||u||_W = \left(\int \left[(1+V(x))^{2\alpha} |u(x)|^2 + \sum_j |\frac{\partial u}{\partial x_j}|^2 dx \right] \right). \tag{5.47}$$

Then, W is a Hilbert space in $L^2(\mathbb{R}^n)$ with compact injection.

Proof. Consider the mapping $p(x) = (1+V(x))^{-\alpha}$. Then $p \in L^\infty(\mathbb{R}^n)$, so that p is a continuous mapping from $H^1(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$. Moreover, $p(x) \to 0$ if $|x| \to \infty$. By Lemma 5.17, multiplication by p is a compact mapping from $H^1(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$. Furthermore, $1/p = (1+V(x))^\alpha \in L^2_{loc}(\mathbb{R}^n)$. We can apply Lemma 5.18 to conclude that W is a Hilbert space in $L^2(\mathbb{R}^n)$ with compact injection. □

We are now in the position to prove Theorem 5.16. We know that the potential is bounded below by some constant $-C$. It is shown in [13] that the domain of the self-adjoint extension is always contained in the form domain $Q(H) := H^1_V(\mathbb{R}^n)$ given by

$$H^1_V(\mathbb{R}^n) = \{u \in W^{1,2}(\mathbb{R}^n) \ | (V+C)^{1/2} u \in L^2(\mathbb{R}^n)\}. \tag{5.48}$$

This set is nothing more than the space V of Corollary 5.19, for $\alpha = 1/2$ and 1 replaced by C. Of course, the latter is just a rescaling and does not change the result. By the same corollary, it now follows that $Q(H)$ is compactly embedded in $L^2(\mathbb{R}^n)$. This proves Theorem 5.16.

This brings us the the next result:

Corollary 5.20. *Let us assume that the injection of $H^1_V(\mathbb{R}^n)$ into $L^2(\mathbb{R}^n)$ is compact. Then $H = -\Delta + V$ has compact resolvent.*

Proof. For $H = -\Delta + V$ and $\lambda \notin \sigma(H)$, the operator $R_\lambda(H) = (\lambda I - H)^{-1}$ is a bijection with continuous inverse $\lambda I - H$. Furthermore, the inclusion map $\iota : H^1_V(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is compact by assumption, and if we restrict it to the domain of H, it is still compact. Now use that the composition of a compact map with a continuous map is compact. Therefore, $R_\lambda(H)$ is compact, and we conclude that H has compact resolvent. □

We apply this corollary to $-\Delta + V$ and conclude that this operator has compact resolvent. Hence Theorem (5.15) has been proven. We need one lemma more to finish step 1.

Lemma 5.21. *An operator with compact resolvent has purely discrete spectrum and therefore has a complete set of eigenfunctions.*

Proof. Let a be an operator with compact resolvent. Then we know by assumption that $b := R_\lambda(a)$ is compact for $\lambda \notin \sigma(a)$. We show first that b^{-1} has discrete spectrum. Note that $0 \notin \sigma(b)$, therefore we may apply the spectral theorem for compact operators to conclude that $\sigma(b)$ consists of countably many non-zero eigenvalues with no accumulation point in $\mathbb{C}$. Since $0 \neq \lambda$ is an eigenvalue of b if and only if λ is an eigenvalue of b^{-1}, we know that $\sigma(b^{-1})$ consists only of eigenvalues which follows from the following observation. If $\lambda \in \rho(b)$, then $b^{-1} - \lambda^{-1}$ is bounded and invertible, since

$$b - \lambda = \lambda b(\lambda^{-1} - b^{-1}), \tag{5.49}$$

so that we have

$$(b^{-1} - \lambda^{-1})^{-1} = -\lambda(b - \lambda)^{-1}b. \tag{5.50}$$

Thus $\lambda^{-1} \in \rho(b^{-1})$. We have showed that $\sigma(b^{-1}) = \{\lambda^{-1} : \ \lambda \in \sigma(b)\}$. As $b^{-1} = a - \lambda$, the above observation implies that a has a discrete spectrum. □

The same result is valid for the operator $\overline{-\Delta + V}$, since the above corollary holds for the closure as well. This proves step 1.

The second step proofs an important fact about strong resolvent convergence of the operator $\overline{-\Delta + V}$. There is another theorem needed that shows essentially self-adjointness of the operator $H = -\Delta + V$ on some domain. The two theorems are given below and can be found in [32, Thm. X.28] and [31, Thm. VIII.25a].

Theorem 5.22. *Let $V \in L^2_{loc}$ with $V \geqslant 0$ pointwise. Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.*

Proof. Put $H = -\Delta + V$. It is clear that H is symmetric, hence closable (with closure $\bar{H} = H^{**}$). Since $V(x) \to +\infty$ if $|x| \to \infty$ and V is bounded from below, we have seen that the corresponding domain of $\bar{H}$ is always contained in the form domain $Q(H) := H^1_V(\mathbb{R}^n)$ given by

$$H^1_V(\mathbb{R}^n) = \{u \in W^{1,2}(\mathbb{R}^n) \ |(V + C)^{1/2}u \in L^2(\mathbb{R}^n)\}. \tag{5.51}$$

Note that $-\Delta + V + 1$ is a strictly positive symmetric operator. Therefore, in view of [32, Thm. X.26], it suffices for self-adjointness of $\bar{H}$ to show that

$$(-\Delta + V + 1)^* u = 0 \implies u = 0, \tag{5.52}$$

for $u \in L^2(\mathbb{R}^n)$ (in the sense of distributions). But $-\Delta + V$ is given with domain $C_0^\infty(\mathbb{R}^n)$, which is dense in $L^2(\mathbb{R}^n)$, so that the above statement is equivalent to

$$(-\Delta + V + 1)u = 0 \implies u = 0 \ \ (u \in L^2(\mathbb{R}^n)). \tag{5.53}$$

Note that $u \in L^2(\mathbb{R}^n)$ and $V \in L^2_{loc}(\mathbb{R}^n)$ imply that $Vu \in L^1_{loc}(\mathbb{R}^n)$. Moreover, $u \in L^1_{loc}(\mathbb{R}^n)$, so that we conclude from the above equality that $\Delta u \in L^1_{loc}(\mathbb{R}^n)$. By Kato's inequality, we have

$$\Delta|u| \geqslant \mathrm{Re}[(\mathrm{sgn}(u))\Delta u] = \mathrm{Re}[(\mathrm{sgn}(u))(V + 1)u] = |u|(V + 1) \geqslant 0. \tag{5.54}$$

In particular, $\Delta|u| \geqslant 0$. Let j_δ be an approximation identity, and $w = |u|$, $w^\delta = w * j^\delta$. It follows from a simple calculation that $\Delta w^\delta = w * \Delta j^\delta \in L^2(\mathbb{R}^n)$. Hence, $w^\delta \in D(\Delta)$. Then,

$$\langle w^\delta, \Delta(w^\delta)\rangle_{L^2} = -\langle \nabla(w^\delta), \nabla(w^\delta)\rangle_{L^2} \leqslant 0, \tag{5.55}$$

with equality only if $w^\delta = 0$. But $\Delta w^\delta = \Delta|u| * j_\delta \geqslant 0$ in distributional sense, hence $\Delta w^\delta \geqslant 0$ pointwise. It follows that $w^\delta = 0$. Using the fact that j_δ is an approximation of the identity, it follows that $\delta \to 0$ implies that $w^\delta \to w$. Therefore, $w = 0$, and hence $u = 0$. □

The next theorem gives a result about strong resolvent convergence:[3]

Theorem 5.23. *Let $\{a_n\}_{n=1}^\infty$ and a be self-adjoint operators and suppose that D is a common core for all a_n and a. If $a_n\varphi \to a\varphi$ for each $\varphi \in D$, then $a_n \to a$ in the strong resolvent sense.*

[3]This notion of convergence is explained in Appendix D (see Definition (D.17)).

Proof. Let $\varphi \in \mathcal{D}$, and put $\mathcal{C} = (a-i)\mathcal{D}$. Note that $\mathcal{C}$ is dense in $\mathcal{H}$, since the deficiency index of $T_{\mathcal{D}}$ is zero, which follows from the fact that a is essentially self-adjoint. Then for each $\varphi \in \mathcal{D}$, we put $\psi = (a-i)\varphi \in \mathcal{C}$. Note that $(a_n - i)^{-1}$ and $(a-i)^{-1}$ exists as i is imaginary and hence is not in the spectrum of a and a_n (since these are self-adjoint). Then:

$$[(a_n - i)^{-1} - (a-i)^{-1}]\psi = \tag{5.56}$$

$$(a_n - i)^{-1}(a-i)\varphi - \varphi = \tag{5.57}$$

$$(a_n - i)^{-1}(a\varphi - i\varphi - a_n\varphi + a_n\varphi) - \varphi = \tag{5.58}$$

$$(a_n - i)^{-1}(a - a_n)\varphi + \varphi - \varphi = \tag{5.59}$$

$$(a_n - i)^{-1}(a - a_n)\varphi. \tag{5.60}$$

By the uniform boundness principle applied to the bounded operators $(a_n - i)^{-1}$, it follows that the $(a_n - i)^{-1}$ are uniformly bounded. Since $(a - a_n)\varphi \to 0$, we can now conclude that the above equation goes to zero if $n \to \infty$. Since $\mathcal{D}$ is dense, we can conclude that

$$(a_n - i)^{-1}\varphi \to (a-i)^{-1}\varphi \quad \forall \varphi \in \mathcal{H}. \tag{5.61}$$

By virtue of [31, Thm. VIII.19], we conclude that we have strong resolvent convergence: $a_n \to a, \quad (n \to \infty)$. □

Then, let $V \in L^2_{\text{loc}}(\mathbb{R}^n)$ be positive and suppose that $\lim_{|x|\to\infty} V(x) = \infty$. Put $V_n = \min\{V, n\}$. Then $\Delta + V_n, -\Delta + V, -\Delta$ and $-\Delta + (V - V_n)$ are essentially self-adjoint on $C_0(\mathbb{R}^n)$ by Theorem 5.22. Moreover, for any $\psi \in C_0(\mathbb{R}^n)$, we clearly have $V_n\psi \to V\psi$ in L^2 as $C_0(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$. Then, by Theorem 5.23 applied to $a_n = \overline{-\Delta + V_n}$ and $a = \overline{-\Delta + V}$, and to $b_n = \overline{-\Delta + (V - V_n)}$ and $b = \overline{-\Delta}$, we have the necessary strong resolvent convergence.

The third step is based on a link giving a connection between the operators $H_0 = -\overline{\Delta}$ and $H = \overline{-\Delta + V}$. Two theorems are needed. The first theorem taken from [33, Thm. XIII.45], is the most important one: it lifts some properties of H_0 to H. The second one is given by a lemma and proves that the properties in question are true for H_0.

Theorem 5.24. *Let H and H_0 be semibounded,[4] self-adjoint operators on $L^2(M, d\mu)$ where $(M, d\mu)$ is a σ- finite measure space. Suppose that there exists a sequence of bounded multiplication operators V_n such that $H_0 + V_n$ converges to H in the strong resolvent sense and so that $H - V_n$ converges to H_0 in strong resolvent sense. Suppose, moreover, that $H - V_n$ and $H + V_n$ are uniforormly bounded from below. Then*

(a) e^{-tH} is positively preserving if and only if e^{-tH_0} is positively preserving.

(b) $\{e^{-tH}\} \cup L^\infty(M, d\mu)$ acts irreducibly on $L^2(M, d\mu)$ if and only if $\{e^{-tH_0}\} \cup L^\infty(M, d\mu)$ acts irreducibly on $L^2(M, d\mu)$.

Proof. Note that the Trotter product formula states that for A and B are self-adjoint operators and $A + B$ is essentially self-adjoint on $\mathcal{D}(A) \cap \mathcal{D}(B)$, then we have

$$\text{s-}\lim_{n\to\infty} (e^{itA/n}e^{itB/n})^n = e^{i(A+B)t}. \tag{5.62}$$

Moreover, if A and B are bounded from below, then

$$\text{s-}\lim_{n\to\infty} (e^{-tA/n}e^{-tB/n})^n = e^{-t(A+B)t}. \tag{5.63}$$

[4]This definition is explained in Appendix D (see Definition (D.14)).

Now, we use the last equality and the continuity of the functional calculus to obtain:

$$e^{-tH} = \text{s-}\lim_{n\to\infty}\left(\text{s-}\lim_{m\to\infty}(e^{-tH_0/m}e^{-tV_n/m})^n\right). \tag{5.64}$$

and

$$e^{-tH_0} = \text{s-}\lim_{n\to\infty}\left(\text{s-}\lim_{m\to\infty}(e^{-tH/m}e^{+tV_n/m})^n\right). \tag{5.65}$$

Since $e^{\pm tV_n/m}$ is positivity preserving, we see that (a) holds. Moreover, by the above two formulas and the fact that $e^{\pm tV_n/m} \in L^\infty(M)$, any subspace left invariant by e^{-tH_0} and $L^\infty(M)$ is left invariant by e^{-tH} and vice versa. Thus no nontrivial closed subspace is left invariant by both e^{-tH} and every bounded multiplication operator, if and only if no nontrivial closed subspace is left invariant by both e^{-tH_0} and every bounded multiplication operator. This proves that $\{e^{-tH_0}\} \cup L^\infty(M, d\mu)$ acts irreducibly on $L^2(M, d\mu)$ if and only if $\{e^{-tH}\} \cup L^\infty(M, d\mu)$ acts irreducibly on $L^2(M, d\mu)$ □

Since the above theorem is based on a proof using the Trotter product formula, which works for self-adjoint operators, we really need H_0 and H_0+V to be self-adjoint. Therefore, we must take their closure, because we know that both operators on the domain $C_0(\mathbb{R}^n)$ are essentially self-adjoint. Thus, using Theorem 5.23 with $a_n = \overline{-\Delta + V_n}$, $a = \overline{-\Delta + V}$, $b_n = \overline{-\Delta + (V - V_n)}$ and $b = \overline{-\Delta}$, where $V_n = \min\{V, n\}$, we have strong resolvent convergence. Moreover, if we can show that the operator e^{-tH_0} is positivity improving, we can indeed apply Theorem 5.24 to conclude that for $H = \overline{-H_0 + V}$, the exponential e^{-tH} is positivity preserving. This will be the next step. We are going to show that for $H_0 = \overline{-\Delta}$, the operator e^{-tH_0} is positivity improving. It follows then by the remark under Theorem 5.11, that it is also ergodic and positivity preserving.

Lemma 5.25. *Given $H_0 = \overline{-\Delta}$, the operator e^{-tH_0} is positivity improving for all $t > 0$.*

Proof. From [32, p.57], we know that $H_0 = \mathcal{F}^{-1}\lambda^2\mathcal{F}$ and $f(H_0) = \mathcal{F}^{-1}f(\lambda^2)\mathcal{F}$, where f is any bounded measurable function. It follows that the operator $e^{-iH_0t} = \mathcal{F}^{-1}e^{-i\lambda^2 t}\mathcal{F}$, for $\text{Im}(t) \leqslant 0$. Theorem IX.29 in [32] states that given $f \in L^\infty(\mathbb{R}^n)$, if either (a) $f \in L^2(\mathbb{R}^n)$ or (b) $\check{f} \in L^1(\mathbb{R}^n)$, then

$$(f(-i\nabla)\varphi)(x) = (2\pi)^{-n/2}\int \check{f}(x-y)\varphi(y)dy, \quad (\varphi \in L^2(\mathbb{R}^n)), \tag{5.66}$$

and the integral converges for all x in case (a) and for almost all x in case (b).

Here, by $f(-i\nabla)$, we denote the operator $\varphi \mapsto \widetilde{(f\widehat{\varphi})}$. With the notation $\widehat{f}$, we mean the Fourier transform $\mathcal{F}(f)$ of f. Similarly, the notation $\check{f}$ means the inverse Fourier transform $\mathcal{F}^{-1}(f)$ of f.

It follows that for $\alpha \in \mathbb{C}$ and $\text{Re}(\alpha) > 0$, we have

$$e^{-\lambda^2\alpha} \in L^\infty(\mathbb{R}^n) \cap L^2(\mathbb{R}^n). \tag{5.67}$$

Therefore, we can apply (5.66) to $e^{-\lambda^2\alpha}$ and we obtain

$$(e^{-H_0\alpha}\varphi)(x) = (4\pi\alpha)^{-n/2}\int e^{\frac{-|x-y|^2}{4\alpha}}\varphi(y)dy \quad (\varphi \in L^2(\mathbb{R}^n)), \tag{5.68}$$

where we used the fact that $\mathcal{F}^{-1}(e^{-\lambda^2\alpha}) = (2\alpha)^{-n/2}e^{-x^2/4\alpha}$.

Now, we are in the position to prove the lemma. We have to show that

$$\langle\psi, e^{-H_0\alpha}\varphi\rangle_{L^2} > 0, \tag{5.69}$$

for all positive functions ψ and φ in $L^2(\mathbb{R}^n)$. By formula (5.68) this is obvious, as $(4\pi\alpha)^{-n/2}e^{\frac{-|x-y|^2}{4\alpha}}$ is strictly positive. For $t > 0$, we put $t = \alpha$, and the statement is of course still true. □

From now on, we will use the notation H_0 to indicate the operator $\overline{-\Delta}$, and H to indicate the operator $\overline{-\Delta + V}$.

As we have just mentioned, it follows that the operator e^{-tH_0} is positivity preserving and ergodic. By Theorem 5.11 $(b) \implies (c)$, we have now that $L^\infty(\mathbb{R}^n) \cup \{e^{-tH_0}\}$ acts irreducibly on $L^2(\mathbb{R}^n)$.

We give a short summary of the steps used as preparation to apply the main Theorem 5.14.

(1) We showed that the spectrum of $H = \overline{-\Delta + V}$ is discrete.

(2) Then we proved that we have strong resolvent convergence so that H_0 and H satisfy the assumptions of Theorem 5.24 with bounded multiplication operators given by $V_n = \min(V, n)$.

(3) It has been shown that e^{-tH_0} is positivity preserving and that $L^\infty(\mathbb{R}^n) \cup \{e^{-tH_0}\}$ acts irreducibly on $L^2(\mathbb{R}^n)$. Thus, by Theorem 5.24, this hold for e^{-tH} as well.

In order to prove that the ground state is strictly positive and non-degenerate, we use Theorem 5.11 applied to our Schrodinger operator H. We know that $-\Delta + V$ is essentially self-adjoint, so that $H = \overline{-\Delta + V}$ is self-adjoint. It is clearly bounded from below:

$$\langle(-\Delta + V)\psi, \psi\rangle = \langle -\Delta\psi, \psi\rangle + \langle V\psi, \psi\rangle \geqslant C||\psi||^2. \tag{5.70}$$

We used that V is bounded from below, and that $-\Delta$ is positive (which follows by Green's identity). Moreover, by scaling the potential we can make $-\Delta+V$ positive. Then, also $H = \overline{-\Delta + V}$ is positive as follows from the next theorem, also stated in Appendix D as Theorem D.13:

Theorem 5.26. *A positive, densely defined, symmetric operator, has a unique positive self-adjoint extension, called the Friedrichs extension.*

Since the operator $-\Delta + V$ is positive, densely defined, and symmetric, the above theorem applies. Since the $-\Delta + V$ is essentially self-adjoint, the extension equals its closure, and it now follows that $\overline{-\Delta + V}$ is positive and thus its spectrum is contained in the positive real axis. In particular, this operator is bounded from below. Since we know by step 1 that the spectrum is discrete, we can now conclude that the bottom of the spectrum of H is an eigenvalue. Hence, by $(a) \iff (c)$ in Theorem 5.11, it suffices to show that e^{-tH} is positivity preserving and that $L^\infty(\mathbb{R}^n) \cup \{e^{-tH}\}$ acts irreducibly. We know these facts for e^{-tH_0} and hence, we may apply Theorem 5.24 to conclude that e^{-tH} is positivity preserving and that $L^\infty(\mathbb{R}^n) \cup \{e^{-tH}\}$ acts irreducibly on $L^2(\mathbb{R}^n)$. We conclude that the ground state of H is non-degenerate and strictly positive. This completes the proof of theorem 5.14.

Consider now the Schrödinger operator with a symmetric double well potential V defined on a domain of $L^2(\mathbb{R})$. Then, it is easy to see that V is in $L^2_{\text{loc}}(\mathbb{R})$, and that $V(x) \to \infty$ as $|x| \to \infty$, by definition of the potential function. Moreover, the potential is bounded below and can always be scaled in order to make it positive. Thus Theorem 5.14 is applicable.

Then finally, consider our Schrodinger operator $\tilde{h}_2 = -\frac{d^2}{dy^2} + V(y)$ with symmetric potential V given by $V(y) = -\frac{1}{2}(2y-1)^2 - \sqrt{(1-y)y}$. We apply Theorem D.19 with $d = 1$ and $\Lambda = [0, 1]$ and V the function given above which is clearly continuous on Λ. The Dirichlet boundary

conditions are given by $V(0) = V(1) = -1/2$. By Theorem D.19, it follows that the spectrum is discrete. The potential is bounded from below and can be translated to make it positive. By a similar argument as for the operator H, also $\overline{-\frac{d^2}{dy^2} + V(y)}$ is positive and has a discrete spectrum, and hence it admits an eigenvalue at the bottom of its spectrum. Furthermore, Theorems 5.22, 5.23, 5.24 and Lemma 5.25 are applicable for the self-adjoint operators $\overline{-\frac{d^2}{dy^2} + V(y)}$, $H_0 \equiv \overline{-\frac{d^2}{dy^2}}$ and e^{-tH_0}. In Theorem 5.24 one can take $V_n = \min(V, \max(V) - \frac{\max(V)}{n})$ in order to get strong resolvent convergence. Thus, by Theorem 5.11 it follows that the ground state of $\tilde{h}_2$ is unique and strictly positive. As expected from numerical simulations and the equivalence established between the scaled quantum Curie-Weiss Hamiltonian J_{N+1}/N and the discretization matrix $\tilde{H}_{N+1}$ (see Chapter 4), this result is in accordance with the fact that the ground state of J_{N+1}/N is unique and strictly positive.

Chapter 6

Classical limit

We have proved in Chapter 3 that the ground state eigenvector $\psi_N^{(0)}$ can be found by diagonalizing the Curie-Weiss Hamiltonian represented with respect to the canonical base of $\mathrm{Sym}^N(\mathbb{C}^2)$. This 'compressed' Hamiltonian was also denoted by J_{N+1}. We have seen in Chapter 4 that the scaled compressed Curie-Weiss Hamiltonian, denoted by J_{N+1}/N, could be viewed as a discretization of a particular Schrödinger operator, which we denoted by $\tilde{h}_2$. Under this identification, it was not clear what the limiting object $\lim_{N\to\infty} J_{N+1}/N$ would be, since the corresponding Schrödinger operator $\tilde{h}_2$ is not defined for $N = \infty$.[1] Therefore, this correspondence only holds semi-classically, in the sense that N needs to be large, but finite. As a result, we could not take the limit of the ground state eigenvector $\psi_N^{(0)}$, at least not naively. The reason for this lies in the fact the limiting system $N \to \infty$ describes a classical theory and rather than a quantum system. The link between the two theories is based on a deformation quantization, in this specific case called Berezin quantization. In order to compute limits, it turns out that we have to transform the ground state eigenvector first into a vector state and then apply this state to the deformation quantization. This method has been extensively studied in [22]. We will discuss this more in detail in §6.3. Regardless of the connection with the Schrödinger operator together with its corresponding classical limit, the Curie-Weiss model also has a classical limit on another algebra, namely on the commutative C^*-algebra $C(B^3)$, with $B^3 \subset \mathbb{R}^3$ the closed unit ball. Again, the relationship between quantum theory and classical theory is described by a deformation quantization map. In the first paragraph of this chapter, we will define this map and give a proof partially based on numerical simulations, showing that the vector state associated to the ground state eigenvector $\psi_N^{(0)}$ of the Curie-Weiss Hamiltonian h_N^{CW} and applied to some deformation quantization, does converge to some probability measure on B^3. We will see that the use of the deformation quantization map plays a crucial role in computing this limit. Hence this map plays a key role in connecting the two different theories (which are individually well-understood).

6.1 Determination of the classical limit

Recall from §3.1 that the local dynamics defined on $B(\mathcal{H}_N) \simeq \bigotimes_{n=1}^N M_2(\mathbb{C}^2)$ is given by

$$\alpha_t^{\Lambda_N}(a) = e^{ith_N^{\mathrm{CW}}} a e^{-ith_N^{\mathrm{CW}}} \qquad (a \in B(\mathcal{H}_N)) \tag{6.1}$$

where h_N^{CW} is the Curie-Weiss Hamiltonian (3.1) defined on the Hilbert space $\mathcal{H}_N = \bigotimes_{n=1}^N \mathbb{C}^2 \simeq \mathbb{C}^{2^N}$. We have seen that the quantum Curie-Weiss model does not converge to a global dynamics on the quasi local C^*- algebra $A = \bigotimes_{x\in\mathbb{Z}} B(H)$, where $H = H_x$ is identified with $\mathbb{C}^2$. However,

[1] Naively (in quantum mechanics) one cannot take the limit $N \to \infty$ (for $\hbar = 1/N$). The limit can however be taken via a detour: deformation quantization. In this case we will see the surprising result that the closed unit ball $B^3 \subset \mathbb{R}^3$ plays a role.

its dynamics does converge to a global dynamics on the commutative C^*-algebra $C(S(B))$, where $B = M_2(\mathbb{C})$ is the single site algebra.

It can be shown by Theorem E.5 from Appendix E that

$$A_0^{(c)} = C(S(M_2(\mathbb{C}))); \tag{6.2}$$

$$A_{1/N}^{(c)} = B(\mathcal{H}_{\Lambda_N}), \tag{6.3}$$

form a continuous bundle of C^*- algebras whose continuous cross-sections are the quasi-symmetric sequences, in this case specified via the symmetrization maps:

$$S_{M,N} : B(\mathcal{H}_{\Lambda_M}) \to B(\mathcal{H}_{\Lambda_N}) \quad (N \geqslant M). \tag{6.4}$$

As a special case for $\mathcal{H}_{\Lambda_M} = \bigotimes_{k=1}^{M} \mathbb{C}^2$ so that $B(\mathcal{H}_{\Lambda_M}) \cong M_2(\mathbb{C})^{\otimes M}$, we have for $N \geqslant M$:

$$S_{M,N} : M_2(\mathbb{C})^{\otimes M} \to M_2(\mathbb{C})^{\otimes N}. \tag{6.5}$$

Regarding $(a_{1/M}) \in B(\mathcal{H}_{\Lambda_M})$ as an element $(a'_{1/M})$ of $B(\mathcal{H}_{\Lambda_M})$ via the canonical embedding $A_{\Lambda_N} \hookrightarrow A_{\Lambda_M}$, we finally define $S_{M,N}$ by

$$S_{M,N}(a_{1/M}) = S_N(a'_{1/M}). \tag{6.6}$$

Here the canonical symmetrizer $S_N : B(\mathcal{H}_{\Lambda_N}) \to B(\mathcal{H}_{\Lambda_N})$ is defined à la (E.21) and (E.22) in Appendix E.

We use the notion of deformation quantization (Appendix E) in order to compute the limit $N \to \infty$ of the N-dependent vector state associated to the ground state eigenvector $\psi_N^{(0)}$ of the system. We shall see that the limit will be a probability measure $\mu_{\psi_N^{(0)}}$ on the Poisson manifold $S(M_2(\mathbb{C})) \cong B^3$. For this, we use the Riesz Representation Theorem, stating that given a compact Haussorff space X, complete regular finite probability measure spaces (X, Σ, μ) uniquely determine a state $\omega : C(X) \to \mathbb{C}$ and vice versa. Given the measure space (X, Σ, μ), then μ defines a state ω by

$$\omega(f) = \int_X d\mu f. \tag{6.7}$$

The converse is more complicated and involves some measure theory. The construction can for example be found in [22, Thm. B.15]. We apply this to $X = B^3$ with ω being a vector state as we will see below.

Denote the deformation quantization map by $Q_N : C(B^3) \to B(\mathcal{H}_N)$, where $N > 0$ is a natural number. Assume first that Q_N is given. Then define

$$\mu_0^{(\infty)}(f) = \lim_{N\to\infty} \omega_0^{(N)}(Q_N(f)) \quad (f \in C(B^3)), \tag{6.8}$$

provided this limit exists . Here, $\omega_0^{(N)}$ is the vector state on $B(\mathcal{H}_N)$ associated to the ground state $\psi_N^{(0)}$, (or more generally to any unit vector in $\mathcal{H}_\mathcal{N}$) given by

$$\omega_0^{(N)}(a_{1/N}) = \langle \psi_N^{(0)}, a_{1/N}\psi_N^{(0)} \rangle \quad (a_{1/N} \in B(\mathcal{H}_N). \tag{6.9}$$

We do not a priori know $Q_N(f)$ for all f on B^3. Fortunately, in view of (E.27), for a fixed M we do have that each $b \in M_2(\mathbb{C})^{\otimes M}$ induces a function $f_b : S(M_2(\mathbb{C})) \cong B^3 \to \mathbb{C}$ given by

$$f_b(\omega) = \lim_{N\to\infty} \omega^N(S_{M,N}(b)) \quad (\omega \in S(M_2(\mathbb{C}))), \tag{6.10}$$

where $S_{M,N} : M_2(\mathbb{C})^{\otimes M} \to M_2(\mathbb{C})^{\otimes N}$ is the symmetrization map, defined for $N \geqslant M$ by (6.5). The above definition makes sense as $S_{M,N}(b)$ is symmetric, and hence quasi-symmetric. Recall from (E.28) that $\omega^N \in S(M_2(\mathbb{C})^{\otimes N})$ is defined as

$$\omega^N(b_1 \otimes \cdots \otimes b_N) = \omega(b_1) \cdots \omega(b_N). \tag{6.11}$$

It follows that

$$f_b(\omega) = \omega^M(b), \tag{6.12}$$

since $N \geqslant M$ and states map the identity element of the operator algebra to the unit element of $\mathbb{C}$. Moreover, f_b is continuous as well.

We define Q_N on these functions f_b induced by b, by

$$Q_N(f_b) = S_{M,N}(b). \tag{6.13}$$

It can be checked that Q_N can indeed be linked to deformation quantization of $X = B^3$ in the sense of Definition E.2. This follows from the fact that the map $0 \mapsto f$ and $1/N \mapsto Q_N \quad (N > 0)$ is a continuous section of the bundle since, by definition of the symmetrization map these clearly form a quasi-symmetric sequence. It is a bit more difficult to check that the Dirac-Groenewold-Rieffel condition (E.6) is satisfied [23]. However, strictly speaking, since the map Q_N has only been defined for these induced functions f_b on B^3, we cannot speak about a deformation quantization. Nonetheless, we will see below that even this partial construction yet provides a very interesting result.
For this, we fix $M = 1$. Then we want to get an indication of what the limit $\mu_0^{(\infty)}$ could be. Since the Pauli matrices together with the identity form a basis for $M_2(\mathbb{C})$, we can just compute $Q_N(f_{\sigma_i})$, where $i = 1, 2, 3$. Denoting $M_2(\mathbb{C})$ by B and recall formula (E.25) from Appendix E:

$$S_{1,N}(\sigma_i) = \frac{1}{N} \sum_{k=1}^{N} \mathbf{1}_B \otimes \cdots \sigma_{i(k)} \otimes \mathbf{1}_B \cdots \otimes \mathbf{1}_B. \tag{6.14}$$

Here k denotes the k^{th} position in the tensor product. It follows that

$$\begin{aligned}
\mu_0^{(\infty)}(f_{\sigma_i}) &= \lim_{N\to\infty} \langle \psi_N^{(0)}, S_{1,N}(\sigma_i)\psi_N^{(0)} \rangle_{\mathcal{H}_N} \\
&= \lim_{N\to\infty} \frac{1}{N} \langle \psi_N^{(0)}, (\sigma_i \otimes 1_B \cdots \otimes 1_B + \cdots + 1_B \otimes \cdots 1_B \otimes \sigma_i)\psi_N^{(0)} \rangle_{\mathcal{H}_N} \\
&= \lim_{N\to\infty} \frac{N}{N} \langle \psi_N^{(0)}, (\sigma_i \otimes 1_B \cdots \otimes 1_B)\psi_N^{(0)} \rangle_{\mathcal{H}_N} \\
&= \lim_{N\to\infty} \mathrm{Tr}_{\mathbb{C}^2}\left[\gamma^{(1)}_{\psi_N^{(0)}} \cdot \sigma_i \right].
\end{aligned} \tag{6.15}$$

In the final last step, we used the fact that $\psi_N^{(0)}$ is a symmetric vector, so that

$$\langle \psi_N^{(0)}, (\sigma_i \otimes 1_B \cdots \otimes 1_B)\psi_N^{(0)} \rangle_{\mathcal{H}_N} = \cdots = \langle \psi_N^{(0)}, (1_B \otimes 1_B \cdots \otimes \sigma_i)\psi_N^{(0)} \rangle_{\mathcal{H}_N}.$$

In the last step we also realize that the inner product equals the trace of the one-particle reduced density matrix associated with the many-particle vector $\psi_N^{(0)}$ called $\gamma^{(1)}_{\psi_N^{(0)}}$, times the spin-Pauli matrix σ_i. A rigorous formalism of this can be found in [25].

The beautiful thing about this link with the reduced density matrix is that the problem

reduces to the computation of the trace of a 2×2-matrix. However, we still need to determine $\gamma^{(1)}_{\psi^{(0)}_N}$. By definition of the one-particle reduced density matrix, the four matrix elements of $\gamma^{(1)}_{\psi^{(0)}_N}$ are given by

$$\left(\gamma^{(1)}_{\psi^{(0)}_N}\right)_{i,j} = \sum_k \langle e_i \otimes \xi_k | \psi^{(0)}_N \rangle \langle \psi^{(0)}_N | e_j \otimes \xi_k \rangle. \tag{6.16}$$

Here $\{\xi_k\}_k$ is an orthonormal basis for $\mathcal{H}_{N-1}$, and $\{e_i\}_{i=1}^2$ is the standard orthonormal basis for $\mathbb{C}^2$.

In order to compute $\mu_0^{(\infty)}(f_{\sigma_i})$, it is necessary to compute the matrix $\gamma^{(1)}_{\psi^{(0)}_N}$. For this, we take the standard orthonormal basis for $\mathcal{H}_{N-1} \cong \mathbb{C}^{2^{N-1}}$. First consider $\left(\gamma^{(1)}_{\psi^{(0)}_N}\right)_{1,1}$. It follows that

$$\left(\gamma^{(1)}_{\psi^{(0)}_N}\right)_{1,1} = \sum_{k=1}^{2^{N-1}} |\langle e_i \otimes \xi_k, \psi^{(0)}_N \rangle|^2. \tag{6.17}$$

Since $\psi^{(0)}_N$ is symmetric, we can write

$$\psi^{(0)}_N = \sum_{n_+=0}^{N} c_{n_+} |n_+, n_- \rangle, \tag{6.18}$$

where $n_+ + n_- = N$, and $|n_+, n_-\rangle$ are the symmetric basis vectors (see also §3.1). These were given by

$$|n_+, n_-\rangle = \frac{1}{\sqrt{\binom{N}{n_+}}} \sum_{l=1}^{\binom{N}{n_+}} \beta_{n_+,l}, \tag{6.19}$$

where, $\beta_{n_+,l}$ are basis vectors for $\mathcal{H}_N \cong \mathbb{C}^{2^N}$ containing n_+- times the vector $e_2 \in \mathbb{C}^2$ in the l^{th} basis vector $\beta_{n_+,l}$ of $\mathcal{H}_N$.

Lemma 6.1. *We have the following identity for the matrix elements of $\gamma^{(1)}_{\psi^{(0)}_N}$:*

$$\left(\gamma^{(1)}_{\psi^{(0)}_N}\right)_{1,1} = \sum_{n_+=0}^{N-1} \frac{c_{n_+}^2}{\binom{N}{n_+}} \binom{N-1}{n_+} = \sum_{n_+=0}^{N-1} c_{n_+}^2 (1 - \frac{n_+}{N}); \tag{6.20}$$

$$\left(\gamma^{(1)}_{\psi^{(0)}_N}\right)_{2,2} = \sum_{n_+=1}^{N-1} \frac{c_{n_+}^2}{1} \frac{n_+}{N} + c_N^2. \tag{6.21}$$

For the off diagonal matrix elements we have:

$$\begin{aligned}
\left(\gamma^{(1)}_{\psi^{(0)}_N}\right)_{1,2} &= \left(\gamma^{(1)}_{\psi^{(0)}_N}\right)_{2,1} \\
&= \sum_{n_+=0}^{N-1} \frac{c_{n_+ +1}\ c_{n_+}}{\binom{N}{n_+ +1}^{1/2} \binom{N}{n_+}^{1/2}} \binom{N-1}{n_+} \\
&= \sum_{n_+=0}^{N-1} \frac{c_{n_+ +1}\ c_{n_+}}{N} (n_+ + 1)^{1/2} (N - n_+)^{1/2}.
\end{aligned} \tag{6.22}$$

Proof. Let $A_k = \{\xi \in H_{N-1} |\ e_2 \ \text{ occurs k times in } \ \xi\}$. Then $\#A_k = \binom{N-1}{k}$. We compute

$$\begin{aligned}\left(\gamma^{(1)}_{\psi_N^{(0)}}\right)_{1,1} &= \sum_{\substack{k=0\\ \xi_k\in A_k}}^{N-1} |\langle e_1\otimes\xi_k, \sum_{n_+=0}^{N}\sum_{l=1}^{\binom{N}{n_+}} \frac{1}{\sqrt{\binom{N}{n_+}}} c_{n_+}\beta_{n_+,l}\rangle|^2 \\ &= \sum_{n_+=0}^{N-1} \frac{c_{n_+}^2}{\binom{N}{n_+}}\binom{N-1}{n_+} \\ &= \sum_{n_+=0}^{N-1} c_{n_+}^2(1-\frac{n_+}{N}). \end{aligned} \tag{6.23}$$

In the second step, we used the fact that $e_1\otimes\xi_k$ and $\beta_{n_+,l}$ are both basis vectors for $\mathbb{C}^{2^{N-1}}$ and that the inner product is orthonormal with respect to these vectors. The last step follows form the identity

$$\frac{\binom{N-1}{n_+}}{\binom{N}{n_+}} = 1-\frac{n_+}{N}. \tag{6.24}$$

Similarly, one can prove that

$$\left(\gamma^{(1)}_{\psi_N^{(0)}}\right)_{2,2} = \sum_{n_+=1}^{N-1}\frac{c_{n_+}^2}{\binom{N}{n_+}}\binom{N-1}{n_+-1} + c_N^2 = \sum_{n_+=1}^{N-1}\frac{c_{n_+}^2}{1}\frac{n_+}{N} + c_N^2. \tag{6.25}$$

It is a bit more difficult to derive a formula for the matrix elements $\left(\gamma^{(1)}_{\psi_N^{(0)}}\right)_{1,2}$ and $\left(\gamma^{(1)}_{\psi_N^{(0)}}\right)_{2,1}$. As before, consider $A_k = \{\xi \in H_{N-1} |\ e_2 \ \text{ occurs k times in } \ \xi\}$. Compute

$$\begin{aligned}\left(\gamma^{(1)}_{\psi_N^{(0)}}\right)_{1,2} &= \sum_k \langle e_1\otimes\xi_k, |\psi_N^{(0)}\rangle\langle\psi_N^{(0)}|e_2\otimes\xi_k\rangle \\ &= \sum_k \langle e_2\otimes\xi_k, \psi_N^{(0)}\rangle\langle e_1\otimes\xi_k, \psi_N^{(0)}\rangle \\ &= \sum_k \langle e_2\otimes\xi_k, \sum_{n_+=0}^{N}\sum_{l=1}^{\binom{N}{n_+}}\frac{1}{\sqrt{\binom{N}{n_+}}}c_{n_+}\beta_{n_+,l}\rangle\langle e_1\otimes\xi_k \sum_{n_+=0}^{N}\sum_{l=1}^{\binom{N}{n_+}}\frac{1}{\sqrt{\binom{N}{n_+}}}c_{n_+}\beta_{n_+,l}\rangle \\ &= \sum_{\substack{k=0\\ \xi_k\in A_k}}^{N-1} \langle e_2\otimes\xi_k, \sum_{n_+=0}^{N}\sum_{l=1}^{\binom{N}{n_+}}\frac{1}{\sqrt{\binom{N}{n_+}}}c_{n_+}\beta_{n_+,l}\rangle\langle e_1\otimes\xi_k \sum_{n_+=0}^{N}\sum_{l=1}^{\binom{N}{n_+}}\frac{1}{\sqrt{\binom{N}{n_+}}}c_{n_+}\beta_{n_+,l}\rangle \\ &= \Big[\frac{c_1}{\binom{N}{1}^{1/2}}\binom{N-1}{0}^{1/2}\Big]\Big[\frac{c_0}{\binom{N}{0}^{1/2}}\binom{N-1}{0}^{1/2}\Big] + \cdots + \\ &\quad \Big[\frac{c_{N-1}}{\binom{N}{N-1}^{1/2}}\binom{N-1}{N-2}^{1/2}\Big]\Big[\frac{c_{N-2}}{\binom{N}{N-2}^{1/2}}\binom{N-1}{N-2}^{1/2}\Big] + c_N\frac{c_{N-1}}{\binom{N}{N-1}^{1/2}} \\ &= \sum_{n_+=0}^{N-1}\frac{c_{n_++1}\ c_{n_+}}{\binom{N}{n_++1}^{1/2}\binom{N}{n_+}^{1/2}}\binom{N-1}{n_+} \\ &= \sum_{n_+=0}^{N-1}\frac{c_{n_++1}\ c_{n_+}}{N}(n_++1)^{1/2}(N-n_+)^{1/2}. \end{aligned} \tag{6.26}$$

The last step follows from an easy computation that uses the identity

$$\frac{1}{\binom{N}{n_++1}^{1/2}\binom{N}{n_+}^{1/2}}\binom{N-1}{n_+} = \frac{1}{N}(n_++1)^{1/2}(N-n_+)^{1/2}. \tag{6.27}$$

By symmetry, using the fact that $\psi_N^{(0)}$ is real-valued, it follows that $\left(\gamma^{(1)}_{\psi_N^{(0)}}\right)_{1,2} = \left(\gamma^{(1)}_{\psi_N^{(0)}}\right)_{2,1}$.

This proves the lemma. □

We have simplified the matrix elements of $\gamma^{(1)}_{\psi_N^{(0)}}$. We are going to prove that $\gamma^{(1)}_{\psi_N^{(0)}}$ converges weakly-$*$ in the trace class sense to $\gamma^{(1)}_\infty$, which is given by

$$\gamma^{(1)}_\infty = \frac{1}{2}\begin{pmatrix} 1 \pm \sqrt{1-B^2} & B \\ B & 1 \mp \sqrt{1-B^2} \end{pmatrix} \quad (0 \leqslant B < 1, J = 1). \tag{6.28}$$

The question is: could we have expected this specific matrix?
The answer is not so difficult, since we know the numerical ground state eigenvector $\psi_N^{(0)}$ of the compressed Curie-Weiss Hamiltonian. We can compute the coefficients easily up to $N = 5000$ using MATLAB. Since this vector is given with respect to the canonical symmetric base for the subspace $\mathrm{Sym}^N(\mathbb{C}^2)$, we have to express $S_{1,N}(\sigma_i) \in \mathcal{H}_N$ in terms of the symmetric basis vectors in order to compute the expression $\langle \psi_N^{(0)}, S_{1,N}(\sigma_i)\psi_N^{(0)} \rangle_{\mathrm{Sym}^N(\mathbb{C}^2)}$ numerically $(i = 1, 2, 3)$. This result in turn will be used to find $\gamma^{(1)}_\infty$.

The following lemma is used to derive an explicit matrix representation for $S_{1,N}(\sigma_i)$ $(i = 1, 2, 3)$, when we represent this operator with respect to the canonical basis for $\mathrm{Sym}^N(\mathbb{C}^2)$.

Lemma 6.2. *In the canonical basis for $Sym^N(\mathbb{C}^2)$, the operator $S_{1,N}(\sigma_3)$ is given by a diagonal matrix with entries on the diagonal*

$$1 - \frac{2i}{N}, \quad (i = 0, ..., N) \tag{6.29}$$

In this basis, the operator $S_{1,N}(\sigma_1)$ has non-zero entries only on the upper and lower diagonal, both given by

$$\sqrt{i(N-(i-1)}/N, \quad i = 1, ..., \lfloor (N+1)/2 \rfloor, \tag{6.30}$$

and for $i = \lfloor (N+1)/2 \rfloor + 1, ..., N+1$, we have

$$\sqrt{(i - \lfloor (N+1)/2 \rfloor (N - (\lfloor (N+1)/2 \rfloor - 1))}/N. \tag{6.31}$$

Here $\lfloor x \rfloor$ denotes the floor function. Thus the lower diagonal equals the upper diagonal, and the entries are repeated in opposite direction at $\lfloor (N+1)/2 \rfloor$.

In this basis the operator $S_{1,N}(\sigma_2)$ only has non-zero entries on the upper and lower diagonal. The lower diagonal is given by the lower diagonal of $S_{1,N}(\sigma_1)$ multiplied with i and the upper diagonal by the upper diagonal of $S_{1,N}(\sigma_1)$ multiplied with $-i$.

Proof. This follows by computing the expressions

$$\langle n_+, n_- | S_{1,N} | (\sigma_i) n_+, n_- \rangle \quad (i = 1, 2, 3), \tag{6.32}$$

with $|n_+, n_-\rangle$ given by (6.19). We omit this computation, as it is similar to the proofs of Theorem 3.1 and Lemma 6.1. □

Using the above lemma, we are finally in the position to compute $\langle \psi_N^{(0)}, S_{1,N}(\sigma_i)\psi_N^{(0)} \rangle_{\mathrm{Sym}^N(\mathbb{C}^2)}$, $(i = 1, 2, 3)$ and show at least numerically that we expect convergence of $\gamma^{(1)}_{\psi_N^0}$ to the specific matrix entries $\left(\gamma_\infty^{(1)}\right)_{i,j}$ as given before by (6.28).
Of course, this inner product is nothing but the scalar inner product on $\mathrm{Sym}^N(\mathbb{C}^2) \cong \mathbb{C}^{N+1}$. It is very easy to compute this inner product numerically. It is not obvious that this will converge as $N \to \infty$, but as we shall see below that, it does though.

We use identity (6.15) and the expressions for $S_{1,N}(\sigma_i)$ that we deduced above and compute

$$\begin{aligned} \mathrm{Tr}_{\mathbb{C}^2}\left[\gamma^{(1)}_{\psi_N^{(0)}} \cdot \sigma_i\right] &= \langle \psi_N^{(0)}, S_{1,N}(\sigma_i)\psi_N^{(0)} \rangle_{\mathrm{Sym}^N(\mathbb{C}^2)} \\ &= \sum_{j=1}^{N+1} \psi_N^{(0)}(j)\overline{(S_{1,N}(\sigma_i)\psi_N^{(0)})(j)}. \end{aligned} \tag{6.33}$$

This sum is computed up to $N = 5000$ $(i = 1, 2, 3)$. The results are given in Figure 6.1 below.

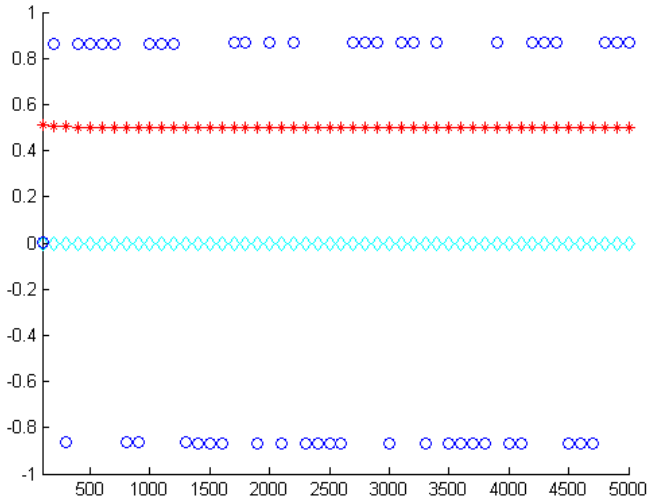

Figure 6.1: The above inner (6.33) *from above has been computed for* $i = 1, 2, 3$*, starting from* $N = 100$ *up to* $N = 5000$*. The blue circles correspond to* $i = 3$*, the red asterisks to* $i = 1$*, and the light blue diamonds to* $i = 2$*. We took* $B = 1/2$ *and* $J = 1$ *in the Curie-Weiss Hamiltonian* (3.1)*.*

The above figure shows that the blue circles that correspond to $i = 3$ are equally and randomly spread over the numbers approximately equal to $\pm\sqrt{3}/2$. This means that the limiting function is double degenerate. It also shows that we have convincing numerical evidence that

$$\mathrm{Tr}_{\mathbb{C}^2}\left[\gamma^{(1)}_{\psi_N^{(0)}} \cdot \sigma_1\right] \to \frac{1}{2}, \tag{6.34}$$

$$\mathrm{Tr}_{\mathbb{C}^2}\left[\gamma^{(1)}_{\psi_N^{(0)}} \cdot \sigma_2\right] \to 0, \tag{6.35}$$

$$\mathrm{Tr}_{\mathbb{C}^2}\left[\gamma^{(1)}_{\psi_N^{(0)}} \cdot \sigma_3\right] \to \pm\frac{\sqrt{3}}{2}. \tag{6.36}$$

Now we are in the position to 'guess' what $\gamma_\infty^{(1)}$ will be.

Since the limiting γ- matrix is still a 2×2- matrix, we can write

$$\gamma_\infty^{(1)} = a_0 \mathbf{1}_2 + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3. \tag{6.37}$$

We know from the above numerical computations that

$$\mathrm{Tr}_{\mathbb{C}^2}\left[\gamma_\infty^{(1)} \cdot \sigma_1\right] = \frac{1}{2}, \tag{6.38}$$

$$\mathrm{Tr}_{\mathbb{C}^2}\left[\gamma_\infty^{(1)} \cdot \sigma_2\right] = 0, \tag{6.39}$$

$$\mathrm{Tr}_{\mathbb{C}^2}\left[\gamma_\infty^{(1)} \cdot \sigma_3\right] = \pm\frac{\sqrt{3}}{2}. \tag{6.40}$$

$$\tag{6.41}$$

Moreover, we have

$$\mathrm{Tr}_{\mathbb{C}^2}\left[\gamma_\infty^{(1)} \cdot \sigma_1\right] = \mathrm{Tr}_{\mathbb{C}^2}\left[(a_0\mathbf{1}_2 + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3) \cdot \sigma_1\right] = 2a_1. \tag{6.42}$$

Similarly, we find that $\mathrm{Tr}_{\mathbb{C}^2}\left[\gamma_\infty^{(1)} \cdot \sigma_2\right] = 2a_2$ and $\mathrm{Tr}_{\mathbb{C}^2}\left[\gamma_\infty^{(1)} \cdot \sigma_3\right] = 2a_3$. Combining this and the above numerical observations, we have

$$\gamma_\infty^{(1)} = \mathbf{1} + \frac{1}{2}\sigma_1 + 0\sigma_2 \pm \frac{\sqrt{3}}{2}\sigma_3, \tag{6.43}$$

as indeed hypothesized for $B = 1/2$. In general, for $0 < B < 1$ and $J = 1$, similar computations can be done and one can show completely analogously that

$$\begin{aligned}\gamma_\infty^{(1)} =& \frac{1}{2}(\mathbf{1} + B\sigma_1 + 0\sigma_2 \pm \sqrt{1-B^2}\sigma_3) \\ =& \frac{1}{2}\begin{pmatrix} 1 \pm \sqrt{1-B^2} & B \\ B & 1 \mp \sqrt{1-B^2} \end{pmatrix},\end{aligned} \tag{6.44}$$

as postulated before by (6.28).

This proof, inspired by numerical computations, shows that

$$\mu_0^{(\infty)}(f_{\mathbf{1}}) = 1 \tag{6.45}$$

$$\mu_0^{(\infty)}(f_{\sigma_1}) = B \tag{6.46}$$

$$\mu_0^{(\infty)}(f_{\sigma_2}) = 0 \tag{6.47}$$

$$\mu_0^{(\infty)}(f_{\sigma_3}) = \pm\sqrt{1-B^2}. \tag{6.48}$$

We will use the isomorphism $S(M_2(\mathbb{C})) \cong B^3$, explicitly given by

$$\omega_{(x,y,z)}(a) = \mathrm{Tr}(\rho(x,y,z)a) \quad ((x,y,z) \in B^3, a \in M_2(\mathbb{C})); \tag{6.49}$$

$$\rho(x,y,z) = \frac{1}{2}\begin{pmatrix} 1+z & x-iy \\ x+iy & 1-z \end{pmatrix}. \tag{6.50}$$

For $b = \sigma_i \ \ (i = 1, 2, 3)$, we use the above isomorphism and equation (6.12) to compute

$$f_{\sigma_i}(\omega_{(x,y,z)}) = \omega_{(x,y,z)}(\sigma_i) = \mathrm{Tr}(\rho(x, y, z)\sigma_i) = f_{\sigma_i}(x, y, z). \tag{6.51}$$

It follows that

$$f_{\mathbf{1}}(x, y, z) = 1; \tag{6.52}$$
$$f_{\sigma_1}(x, y, z) = x; \tag{6.53}$$
$$f_{\sigma_2}(x, y, z) = y; \tag{6.54}$$
$$f_{\sigma_3}(x, y, z) = z. \tag{6.55}$$

Denoting the point $(B, 0, \pm\sqrt{1 - B^2})$ by $x_\pm$, we then have

$$f_{\mathbf{1}}(x_\pm) = 1 \tag{6.56}$$
$$f_{\sigma_1}(x_\pm) = B; \tag{6.57}$$
$$f_{\sigma_2}(x_\pm) = 0; \tag{6.58}$$
$$f_{\sigma_3}(x_\pm) = \pm\sqrt{1 - B^2}. \tag{6.59}$$

It is known [22, Sec. 10.8] (and easy to verify) that the classical Curie-Weiss Hamiltonian on B^3, given by

$$h^{\mathrm{CW}}_\infty(x, y, z) = -\frac{1}{2}z^2 - Bx, \tag{6.60}$$

has a doubly degenerate ground state for $0 < B < 1$, given by

$$x_\pm = (B, 0, \pm\sqrt{1 - B^2}). \tag{6.61}$$

In view of the proof of Lemma 2.5 in Chapter 2, we know that the points $x_\pm$ correspond to Dirac measures $\tilde{\mu}^\pm_0$ (or, equivalently, to pure states), given by:

$$\tilde{\mu}^\pm_0(f) := \delta_{(B,0,\pm\sqrt{1-B^2})}(f) = \int_{B^3} d\tilde{\mu}_{(B,0,\pm\sqrt{1-B^2})}(f) = f(B, 0, \pm\sqrt{1 - B^2}) \ \ (f \in C(B^3)). \tag{6.62}$$

From the above equation, using f_b for $b = \sigma_i \ \ (i = 1, 2, 3)$, we recover precisely equations (6.46)-(6.48). In fact, we have numerically proven that for a specific choice of the deformation quantization acting on the functions f_b coming from a matrix $b \in M_2(\mathbb{C})$, namely $Q_N(f_b) = S_{1,N}(b)$, the limit defined in (6.8) exists and is precisely the doubly degenerate ground state that corresponds to the classical Hamiltonian h^{CW}_∞ (for $0 < B < 1$ and $J = 1$). The ensuing $\mathbb{Z}_2$-symmetry on B^3 is simply given by the map $(x, y, z) \mapsto (x, -y, -z)$. From a similar argument as given in the text under Lemma 2.5, one can show that the degenerate (pure) ground states $\tilde{\mu}^\pm_0$ on $C(B^3)$ are not $\mathbb{Z}_2$-invariant, so that the symmetry is spontaneously broken.
This is completely in accordance with the link between the Curie-Weiss model and the corresponding Schrödinger operator. We have seen in §4.6 that for $0 < B < 1$ we obtained a double well potential such that in the classical limit the ground state was doubly degenerate and displayed SSB, even though these ground states were defined on a different algebra from the one we just considered, namely $C(B^3)$. This will become clearer in §6.3.

Remark.
We haven't made a clear distinction between convergence of the delocalized eigenvectors $\psi^{(0)}_N$ and $\psi^{(1)}_N$, or the localized eigenvectors $\frac{1}{\sqrt{2}}(\psi^{(0)}_N \pm \psi^{(1)}_N)$. For the double well, it known that the delocalized wave functions converge to a mixed state on the corresponding classical algebra. The localized

wave functions, which define pure states as well, converge to pure states on this algebra [22], [34]. The latter states indeed correspond to Dirac measures. As for the double well, we can expect a similar result for the Curie-Weiss model. However, we could not check this for the delocalized eigenvectors $\psi_N^{(0)}$ and $\psi_N^{(1)}$, since due to numerical inaccuration these already localize for $N \approx 80$. As a result, we expect convergence to a pure classical state. Fortunately, we already found this correct outcome.

6.2 Convergence of the reduced density matrix

In this section we say more about the convergence of the matrix $\gamma^{(1)}_{\psi_N^{(0)}}$ to the matrix $\gamma_\infty^{(1)}$. It is extremely difficult to prove this analytically, since the ground state eigenvector $\psi_N^{(0)}$ is only given numerically, being a solution of the characteristic equation corresponding to the smallest eigenvalue.

We have seen in Chapter 4 that for large but finite N, the compressed (scaled) Hamiltonian that we denoted by J_{N+1}/N was in some sense equivalent to a discretization of the Schrödinger operator $\tilde{h}_2$ on $L^2([0,1])$ describing a particle in a one-dimensional symmetric double well.
We have also seen that the lowest eigenfunctions of such a Schrödinger operator with a symmetric double well potential are approximately given by linear combinations of the weighted Hermite polynomials (see §3.2). In particular, for N large enough, the ground state was approximately given by a linear combination of Gaussians

$$\frac{T_a(\varphi_0) + T_{-a}(\varphi_0)}{\sqrt{2}}, \tag{6.63}$$

where the symbol $\pm a$ indicates the position on both minima of the symmetric double well potential and $T_{\pm a}$ is the translation operator over distance $\pm a$, i.e., $(T_{\pm a}\varphi_0)(x) = \varphi_0(x \pm a)$.

In our previous discussion in Chapter 4 it was not clear what the limiting object $\lim_{N\to\infty} J_{N+1}/N$ would be, since the corresponding Schrödinger operator $\tilde{h}_2$ was not defined for $N = \infty$. As a result,[2] we could not just take the limit $N \to \infty$ of the ground state eigenvector $\psi_N^{(0)}$. We will see in §6.3 that the so-called Berezin quantization is involved when computing the classical limit of this Schrödinger problem. Nonetheless, we have already seen that the use of the deformation quantization map defined in the beginning of the previous paragraph enables us to speak about the limit (6.8), which will be different than the one for the Schrödinger operator. This limit was a probability measure on the compact space B^3, at least defined for special functions f_b.

In §4.7 we argued that, when discretizing the grid, the number of points in this peak increases with $\sqrt{N}$, so that the in fact we get a better approximation of this Gaussian, as we also have observed numerically. The next step is then to fit the numerical vector components c_{n_+} to Gaussians. Following this approach, one can try to use these Gaussians rather then only the numerical values c_{n_+} in order to compute the limit $N \to \infty$ of equation (6.8). The idea is to prove things more analytically using these Gaussian functions, rather then only numerical values.
We are going to fit our numerical ground state eigenvector $\psi_N^{(0)}$ to a Gaussian $G_N^{(0)}$ using MATLAB. This time for simplicity, we take the operator J_{N+1} rather than the scaled one, since the eigenvectors do not change by a scaling constant. We will show analytically that, using these fitted Gaussians instead of the numerical vector $\psi_N^{(0)}$, the matrix $\gamma^{(1)}_{G_N^{(0)}}$ indeed converges to $\gamma_\infty^{(1)}$.

[2]Note that for any finite N the ground state eigenvector, seen as the original eigenvector of the Curie-Weiss model or as the eigenvector of the discretization matrix $\tilde{H}_N$ of the Schrödinger operator $\tilde{h}_2$ is well-defined and independent of the type of classical limit we take, which depends only on the deformation quantization. However, inspired by Chapter 4, we know that the ground state looks like a Gaussian, and thus we will fit $\psi_N^{(0)}$ to a Gaussian.

The mixed ground state $\frac{1}{\sqrt{2}}(T_a\varphi + T_{-a}\varphi)$ is never seen numerically for $N \geqslant 80$, as explained in Chaper 3 and 4. Hence we fit $\psi_N^{(0)}$ to $T_{\pm a}\varphi$. By symmetry, we can restrict to only $T_a\varphi$. We fit the ground state eigenvector $\psi_N^{(0)}$ on the discrete grid $[0 : \Delta : 1]$ (with uniform grid spacing $\Delta = 1/N$) to the Gaussian in the most general form:

$$G_N^{(0)}(x) = a_1 e^{(-((x-b_1)/c_1)^2)} \tag{6.64}$$

A plot of this fit is displayed in Figure 6.2.

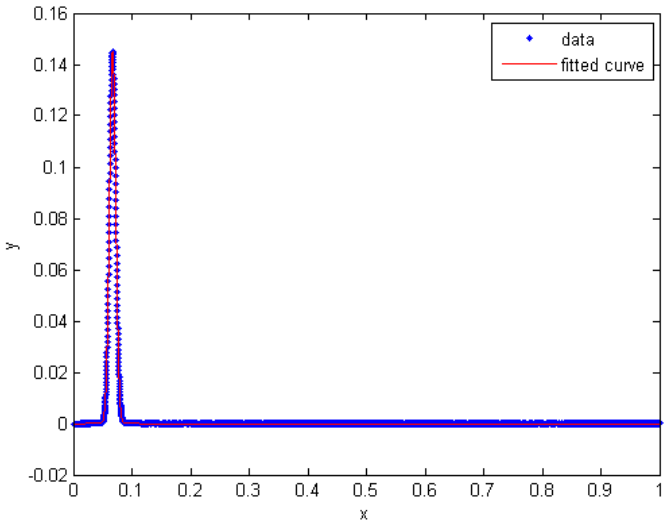

Figure 6.2: The ground state eigenvector $\psi_N^{(0)}$ fitted to the above Gaussian for $N = 5000$.

As we have seen, the eigenvector will be numerically degenerate, so that we indeed observe one peak instead of two. For this value of $N = 5000$, we find the following values for the fit parameters:

Fit parameters	
parameters	value
a_1	0.1449
b_1	0.06702
c_1	0.007597

Of course, these parameters depend on N. However, the position of the maximum indicated by b_1 tends to converge to a fixed value being $0.0670 \approx B(1-\sqrt{1-B^2})$, for $B = 1/2$. This result is purely based on numerics. By symmetry, the other maximum is then given by $1 - b_1 = B(1 + \sqrt{1-B^2})$. When one compares these two values to the double well as given in (4.90), they indeed correspond to both minima of this potential, given by $B(1 - \sqrt{1-B^2})$ and $1 - B(1 - \sqrt{1-B^2})$. The other parameters are more difficult to handle since the amplitude and the width of the Gaussian depend on N, and we may not speak about the limit of the single Gaussian. However, we can always try to prove that $\gamma^{(1)}_{G_N^{(0)}}$ converges to matrix $\gamma_\infty^{(1)}$ as $N \to \infty$, (but $N \neq \infty$, which is undefined). This will be the next step.

We have deduced the entries of $\left(\gamma^{(0)}_{\psi^{(0)}_N}\right)_{i,j}$ for $\psi^{(0)}_N$. The same formulas of course holds for the fitted Gaussian $G^{(0)}_N$. We find on the grid $[0:1/N:1]$:

$$\left(\gamma^{(0)}_{\psi^{(0)}_N}\right)_{1,1} \approx \sum_{n_+=0}^{N-1} (G^{(0)}_N(n_+/N))^2(1-\frac{n_+}{N}) \tag{6.65}$$

$$= \sum_{n_+=0}^{N-1} (G^{(0)}_N(n_+/N))^2 - \sum_{n_+=0}^{N-1} (G^{(0)}_N(n_+/N))^2\frac{n_+}{N}. \tag{6.66}$$

Using the fact that $\psi^{(0)}_N$ is normalized, also the fitted Gaussian $G^{(0)}_N$ will be normalized to a good approximation. So when we take N large enough, the first term converges to 1. An outline of a proof of convergence is as follows. Consider the first term. The function

$$\frac{1}{N}\sum_{n_+=0}^{N-1} (G^{(0)}_N(n_+/N))^2 \tag{6.67}$$

is the Riemann sum for the function $(G^{(0)}_N(x))^2$ over the interval $x \in (0,1)$. Hence, for N large, the original sum behaves like

$$N\int_0^1 (G^{(0)}_N(y))^2 dy = \frac{Na_1^2\sqrt{2\pi}c_1}{4}\left[\mathrm{erf}(\frac{1-b_1}{\sqrt{2}c_1/2}) - \mathrm{erf}(\frac{0-b_1}{\sqrt{2}c_1/2})\right]. \tag{6.68}$$

However, the function $(G^{(0)}_N(x))^2$ is almost zero outside the interval $(0,1)$ since the Gaussian function decays exponentially. For $N = 5000$, the value at the boundary is of the order 10^{-45}. Thus, it is reasonable to integrate over the whole real axis to find that

$$N\int_{-\infty}^{\infty} (G^{(0)}_N(y))^2 dy = Na_1^2\sqrt{2\pi}c_1/2 \approx 0.9993 \approx 1. \tag{6.69}$$

Here, we used that $\int_{-\infty}^{\infty}(G^{(0)}_N(y))^2dy = \frac{\sqrt{2\pi}c_1}{2}$.

Now consider the second term. Using $n_+ = \frac{Nn_+}{N}$, for large N, the function

$$-\frac{1}{N}\sum_{n_+=0}^{N-1}\frac{Nn_+}{N}(G^{(0)}_N(n_+/N))^2 = -\sum_{n_+=0}^{N-1}\frac{n_+}{N}(G^{(0)}_N(n_+/N))^2 \tag{6.70}$$

corresponds to the integral over the interval $(0,1)$ given by

$$-N\int_0^1 y(G^{(0)}_N(y))^2 dy. \tag{6.71}$$

As before, already for $N = 5000$ the function value of the exponential $G^{(0)}_N$ on the boundary is of the order 10^{-45}, so that multiplication by the function y does change this order, as the latter function increases more slowly to infinity than the exponential decreases to zero. Hence we can take the integration domain to be the whole real line. That gives

$$-N\int_{-\infty}^{\infty} y(G^{(0)}_N(y))^2 dy = Na_1^2\sqrt{2\pi}\frac{c_1}{2}b_1 \approx -b_1. \tag{6.72}$$

This shows that for $N = 5000$, we find that (still using $B = 1/2$ and $J = 1$)

$$\left(\gamma^{(1)}_{G^{(0)}_N}\right)_{1,1} \approx 1 - b_1 \approx B(1 + \sqrt{1 - B^2}). \tag{6.73}$$

Completely similarly to the previous one, we get

$$\left(\gamma^{(1)}_{G^{(0)}_N}\right)_{2,2} \approx \sum_{n_+=1}^{N-1} \frac{(G^{(0)}_N(n_+/N)^2}{1} \frac{n_+}{N} + G^{(0)}_N(1))^2. \tag{6.74}$$

Using $G^{(0)}_N(1))^2 \approx 0$, we find that

$$\left(\gamma^{(1)}_{G^{(0)}_N}\right)_{2,2} \approx b_1 \approx B(1 - \sqrt{1 - B^2}). \tag{6.75}$$

This brings us to the final two equations $\left(\gamma^{(1)}_{G^{(0)}_N}\right)_{1,2} = \left(\gamma^{(1)}_{G^{(0)}_N}\right)_{2,1}$, where again we used the fitted Gaussian for $\psi^{(0)}_N$.

Unfortunately, these equations are more difficult to handle since they involve the function $\frac{\sqrt{n_++1}\sqrt{N-n_+}}{N}$. We can rewrite the product $G^{(0)}_N(n_+ + 1)G^{(0)}_N(n_+)$ in terms of one single Gaussian. For $j \in [0 : 1/N : 1]$, by completing the square we find that

$$\begin{aligned} G^{(0)}_N(j+1)G^{(0)}_N(j) =& a_1^2 e^{(-(((j+1)-b_1)/c_1)^2)} e^{(-((j-b_1)/c_1)^2)} \\ =& a_1^2 e^{-\frac{2}{N^2c_1^2}\left(j - \frac{\frac{4b_1}{N} - \frac{2}{N^2}}{\frac{4}{N^2}}\right)^2} e^{-\frac{1}{c_1^2}\left(\frac{1}{N^2} - \frac{2b_1}{N} + 2b_1^2 - \frac{(\frac{2}{N^2} - \frac{4b_1}{N})^2}{8/N^2}\right)}. \end{aligned} \tag{6.76}$$

The function

$$\frac{1}{N}\sum_{n_+=0}^{N-1} \sqrt{N - n_+}\sqrt{n_+ + 1} G^{(0)}_N((n_+ + 1)/N) G^{(0)}_N(n_+/N) \tag{6.77}$$

is the Riemann sum for the function above function on the interval $(0, 1)$. Hence for N large, this behaves like the integral

$$a_1^2 e^{-\frac{1}{c_1^2}\left(\frac{1}{N^2} - \frac{2b_1}{N} + 2b_1^2 - \frac{(\frac{2}{N^2} - \frac{4b_1}{N})^2}{8/N^2}\right)} \int_0^1 e^{-\frac{2}{N^2c_1^2}\left(y - \frac{\frac{4b_1}{N} - \frac{2}{N^2}}{\frac{4}{N^2}}\right)^2} \sqrt{N - Ny}\sqrt{Ny + 1} dy. \tag{6.78}$$

This integral indicates the expectation value of the function $\sqrt{N - Ny}\sqrt{Ny + 1}$ over the interval $(0, 1)$ that corresponds to the density function given by the Gaussian

$$e^{-\frac{2}{N^2c_1^2}\left(y - \frac{\frac{4b_1}{N} - \frac{2}{N^2}}{\frac{4}{N^2}}\right)^2}. \tag{6.79}$$

We computed $\left(\gamma^{(1)}_{G^{(0)}_N}\right)_{1,2}$ for $N = 5000$, obtaining

$$\left(\gamma^{(1)}_{G^{(0)}_N}\right)_{1,2} \approx 0.2501 \approx 1/4 = \frac{B}{2}. \tag{6.80}$$

We conclude that using these Gaussians, the matrix $\gamma^{(1)}_{G^{(0)}_N}$ converges to $\gamma^{(1)}_\infty$.

This result, inspired by numerical evidence as well as by the link between our system and the harmonic oscillator, is based on the fact that we could fit the ground state eigenvector $\psi^{(0)}_N$ to a Gaussian $G^{(0)}_N$, for N large enough. We have already shown numerically that $\gamma^{(1)}_{\psi^{(0)}_N}$ converges to $\gamma^{(1)}_\infty$. However, using these Gaussians instead, we showed that the same result is true and is not based on pure numerical computations.

We still need to understand in which sense we have convergence.[3] We claim that the convergence of states is in the sense of the weak* topology defined by the duality $B_1(\mathcal{H}) \cong B_0(\mathcal{H})^*$. This means that given a sequence $(T_n)_n \in B_1(\mathcal{H})$ of trace-class operators[4] and a $T \in B_1(\mathcal{H})$, we have[5]

$$T_n \to T \ \ (\text{weak}^*) \iff \forall J \text{compact} : \text{Tr}(JT_n) \to \text{Tr}(JT) \ \ (n \to \infty). \tag{6.81}$$

In our case $\mathcal{H} = \mathbb{C}^2$, so that the Pauli spin matrices together with the identity matrix form a basis for $M_2(\mathbb{C})$, as we have also seen before. Therefore, showing that

$$\text{Tr}_{\mathbb{C}^2}(\gamma^{(1)}_{\psi^{(0)}_N}\ \sigma_i) \to \text{Tr}_{\mathbb{C}^2}(\gamma^{(1)}_\infty\ \sigma_i) \tag{6.82}$$

proves that

$$\gamma^{(1)}_{\psi^{(0)}_N} \to \gamma^{(1)}_\infty \ \ (\text{weak}^*). \tag{6.83}$$

This is exactly what we have just shown.

6.3 Two classical limits

In the previous two paragraphs, we have shown that the vector state associated to the ground state eigenvector[6] $\psi^{(0)}_N$ converges to a doubly degenerate Dirac measure on B^3. We needed a deformation quantization map in order to make this work. In Chapter 4, we linked our compressed Curie-Weiss Hamiltonian to a Schrödinger operator with a symmetric double well potential. Also the ground state of this Hamiltonian has a classical limit, as we will explain briefly below.

We know from the example in Appendix E that there exists a deformation quantization of $\mathbb{R}^2$, called Berezin quantization: $Q^B_\hbar : C_0(\mathbb{R}^2) \to B_0(L^2(\mathbb{R}))$, and defined by equation (E.15). Consider then the Hamiltonian $h_\hbar$ with a symmetric double well potential, defined on $L^2(\mathbb{R})$. It has been shown that using Berezin quantization, the localized wave functions of this Hamiltonian converge to some double degenerate Dirac measure on $\mathbb{R}^2$ [22], [34]. These Dirac measures are given by

$$\int_{\mathbb{R}} d\mu^\pm_0 f = f(0, \pm a), \tag{6.84}$$

[3]The space $B_1(\mathcal{H})$ is the set of trace-class operators, and the space $B_0(\mathcal{H})^*$ denotes the dual space of the compact operators. Here, the symbol $\cong$ stands for isometric isomorphism, given by the map $B_1(\mathcal{H}) \to B_0(\mathcal{H})^*$, $u \mapsto \text{Tr}(u\cdot)$ ($u \in B_1(\mathcal{H})$). A proof of this result can for example be found in [22].

[4]A trace-class operator is an operator a such $\text{Tr}(|a|)$ is finite.

[5]Let X be a normed vector space. A net (φ_λ) of functionals in X^* converges to a functional $\varphi \in X^*$ in the weak* topology if $\varphi_\lambda(a) \to \varphi(a)\ \forall a \in X$. In this case $B_1(\mathcal{H}) \cong B_0(\mathcal{H})^*$ under the map $u \mapsto \text{Tr}(u\cdot)$. Then weak* convergence of a net $(u_\lambda) \in B_1(\mathcal{H})$ to an operator $u \in B_1(\mathcal{H})$ is equivalent to saying $\text{Tr}(u_\lambda a) \to \text{Tr}(ua)\ \forall a \in B_0(\mathcal{H})$.

[6]This holds only for the localized eigenvectors. Due to numerical degeneracy, the ground state $\psi^{(0)}_N$ will be automatically localized for $N \geqslant 80$, so that the classical limit will be indeed a pure state.

where $\pm a$ denotes the position of the left and right minimum of the potential. Lemma 2.5 showed that these measures break the $\mathbb{Z}_2$-symmetry in sense of Definition 2.3. Moreover, in a similar way, we can define the Berezin quantization of $[0,1]\times\mathbb{R}$.[7] We then get

$$Q_\hbar^B : C_0([0,1]\times\mathbb{R}) \to B_0(L^2([0,1])), \tag{6.85}$$

defined by (E.15) as well. If we now consider the Schrödinger operator $\tilde{h}_2$ from equation (4.89), then one can analogously show that its (vector) state associated to the ground state eigenfunction $\psi_N^{(0)}$, now corresponding to $\tilde{h}_2$, converges to a symmetric sum of Dirac measures on $[0,1]\times\mathbb{R}$. These measures then correspond to the points $(B(1\pm\sqrt{1-B^2}),0)$, where $B(1\pm\sqrt{1-B^2})$ are precisely the minima of the potential double well. The proof of this is similar to the one for the Curie-Weiss model (explained in §6.1), with one detail different. We are given the discrete eigenvector $\psi_N^{(0)}$ that corresponds to $\tilde{H}_N$, i.e., the discretization of $\tilde{h}_2$. We should approximate the integral (E.15) by a sum, and put $\hbar = 1/N$. Then it is a matter of computing $\langle\psi_N^{(0)}, Q_{1/N}^B(f)\psi_N^{(0)}\rangle$, given by equation (E.16). Since for N sufficiently large, our vector $\psi_N^{(0)}$ behaves like a delta-peak concentrated in both minima of the well, it is obvious that (E.16) will converge to the function $f(B(1\pm\sqrt{1-B^2}),0)$.

On the one hand, using the deformation quantization Q^N of B^3 defined in §6.1, we have a classical limit of the ground state associated to the eigenvector $\psi_N^{(0)}$, originally corresponding to the Curie-Weiss Hamiltonian. On the other hand, making the identification with the Schrödinger operator and using the Berezin quantization of $[0,1]\times\mathbb{R}$, it follows that the same ground state, but now applied to this map, has a classical limit as well. Both different classical limits therefore consist of a doubly degenerate ground state that break the $\mathbb{Z}_2$-symmetry (in the regime $0<B<1$).

6.4 The Lipkin-Meshkov-Glick (LMG) Model

In this section we consider the Lipkin-Meshkov-Glick Model which is a generalization of the Curie-Weiss model under some transformation.
The Lipkin-Meshkov-Glick Model, or LMG model, was first proposed to describe phase transitions in atomic nuclei [24]. We will focus on the spontaneous symmetry breaking, which has already been studied by for many years in this model, see for example [3]. Recently, it was found that the LMG model is relevant to many other quantum systems, such as cavity QED [27].

The Hamiltonian of a general LMG model is given by

$$h_N^{LMG} = \frac{\lambda}{N}(S_1^2 + \gamma S_2^2) - BS_3, \tag{6.86}$$

where $S_i = \sum_x \sigma_i(x)/2$ is the total spin operator summing over all N spins, and σ_i is the i^{th} spin Pauli matrix. We are interested in $\lambda < 0$, standing for a ferromagnetic interaction, $\gamma \in (0,1]$ describing the anisotropic in-plane coupling, and B is the magnetic field along z direction with $B \geqslant 0$. Also recall that for $\lambda = -1$ it is well known that a quantum phase transition occurs at $B = 1$ [17]. Note that the LMG-model is just the Curie-Weiss model for $\gamma = 0$, and the transformation $\sigma_1 \mapsto \sigma_3$ and $\sigma_3 \mapsto \sigma_1$.

We will focus on the regime $0 \leqslant B < 1$ with $\lambda = -1$.

[7] The set $[0,1]$ denotes the configuration space, i.e., the space of all possible 'positions' of the system. The set $\mathbb{R}$ is the momentum space, i.e., the space of all possibile 'momenta' of the system. The cotangent bundle of the configuration space $T^*Q \cong [0,1]\times\mathbb{R}$ is called the phase space, incorporating all possible positions and momenta of the system.

First consider $\gamma = 1$, called the isotropic case. Based on [17], it has been shown that the eigenenergies of the isotropic Hamiltonian are given by

$$E(S, M) = -\frac{1}{N}[S(S+1) - M^2] - BM. \tag{6.87}$$

Moreover, the ground state localizes at $S_0 = N/2$ and

$$M_0 = \begin{cases} \lfloor \frac{BN}{2} \rfloor, & \text{for } N \text{ even} \\ \lfloor \frac{BN}{2} + \frac{1}{2} \rfloor - \frac{1}{2}, & \text{for } N \text{ odd} \end{cases} \tag{6.88}$$

Here, $\lfloor \cdot \rfloor$ denotes the floor function.

Observe that the Hamiltonian h_N^{LMG} commutes with the Symmetrizer operator, for any $\gamma \in [0, 1]$. We want the ground state to be in the range of the Symmetrizer operator in order to diagonalize the matrix with respect to the canonical base for $\mathrm{Sym}^N(\mathbb{C}^2)$. As we have seen many times before since both operators commute, a sufficient condition for the ground state being in the range of the Symmetrizer is uniqueness. For the Curie-Weiss model, this is shown by the Perron-Frobenius Theorem. When we write the LMG Hamiltonian with respect to the standard basis for $\otimes_{n=1}^N \mathbb{C}^2 \cong \mathbb{C}^{2^N}$, its corresponding matrix is not positive definite. In fact, it has strictly positive as well as strictly negative entries. Therefore, the Perron-Frobenius Theorem is not applicable to this matrix. However, based on numerical intuition, the ground state will be in the range of the Symmetrizer even though it might be not unique as we will see. We have diagonalized the LMG Hamiltonian up to $N = 15$, by writing the Hamiltonian with respect to the standard basis for $\mathbb{C}^{2^N}$ and comparing the ground state eigenvalue to the one obtained when diagonalizing the matrix with respect to the symmetric basis for $\mathrm{Sym}^N(\mathbb{C}^2)$. We observed that for these values of N the ground state eigenvalues are the same for both (independent) diagonalization processes. Therefore, we may conclude that at least for these values of N, the ground state indeed lies in this subspace, and therefore is symmetric.

It is not difficult to show that the matrix entries of h_N^{LMG} written with respect to the symmetric basis are located on the diagonal and given by

$$\langle n_+ n_-, h_N^{\mathrm{LMG}} n_+ n_- \rangle = -\frac{1}{4}(2(N + 2n_- n_+)) - \frac{B(n_+ - n_-)}{2}. \tag{6.89}$$

Assuming for a moment that the ground state eigenvector lies in this subspace, then clearly it will be a (canonical) basis vector, since the Hamiltonian represented in this subspace is a diagonal matrix. Therefore, in order to compute this eigenvector we just have to solve the following equation for n_+:

$$E(N/2, M_0) = -\frac{1}{4}(2(N + 2n_- n_+)) - \frac{B(n_+ - n_-)}{2}. \tag{6.90}$$

It is not difficult to show that for any N there are two solutions for n_+:

$$n_+^1 = N - \lfloor \frac{N}{4} \rfloor; \quad \text{and} \tag{6.91}$$

$$n_+^2 = \frac{N}{2} + \lfloor \frac{N}{4} \rfloor. \tag{6.92}$$

This also shows that the ground state is double degenerate when $n_+^1 \neq n_+^2$. We conclude that if the ground state eigenvector lies in the symmetric space, it is given by n_+^1 or n_+^2 and could therefore be degenerate in contrast to the finite quantum Curie-Weiss model.

Consider now the anisotropic case, for $\gamma \neq 1$. In contrast to the anisotropic LMG model, it it has been proved that the ground state of the isotropic LMG model in the limiting mean field is infinitely degenerate [8]. It has also been explained in [8] that for $\gamma \in [0,1)$ and $\lambda = -1$ the ground state of (6.86) is non-degenerate for any finite N, and hence unique. Again, this does not easily follow from the Perron-Frobenius theorem applied to the matrix written with respect to the standard basis. Since we still know that the anisotropic Hamiltonian commutes with the Symmetryzer, it follows that for any finite N the ground state of the anisotropic LMG model ($\lambda = -1$) lies in the range of the symmetrizer operator. Without loss of generality, this allows us to diagonalize the anisotropic LMG Hamiltonian ($\lambda = -1$) with respect to $\mathrm{Sym}(\mathbb{C}^2)$. Similar to Theorem 3.1 we deduce a formula for the matrix entries for this Hamiltonian.

Lemma 6.3. *In the symmetric basis, the LMG-Hamiltonian h_N^{LMG} given in equation* (6.86) *for $\gamma \in [0,1)$ and $\lambda = -1$ is a tridiagonal matrix with diagonal entries given by*

$$-\frac{1}{4}(n_+(n_- + 1) + n_-(n_+ + 1))(1+\gamma) - \frac{B}{2}(n_+ - n_-), \tag{6.93}$$

and on the second upper and second lower diagonal we have

$$-\frac{1}{4}\sqrt{(n_+ + 2)(n_+ + 1)}\sqrt{(n_-)(n_- - 1)}(1-\gamma). \tag{6.94}$$

Thus the only non-zeros entries are located on the diagonal and on the second upper and lower diagonal, i.e the elements $(i, i+2)$ and $(i+2, i)$.

Proof. The proof is similarto the proof of Theorem 3.1 for the Curie-Weiss Hamiltonian, and is therefore omitted. □

The next step is to define a deformation quantization map that we can apply to the ground states of the anisotropic LMG Hamiltonian ($\lambda = -1$) in order to compute limits. We took the same deformation quantization map as for the Curie-Weiss model, i.e., $Q_N(f_b) = S_{1,N}(b)$, where $b \in M_2(\mathbb{C}^2)$, where the classical C^*-algebra is still given by $C(B^3)$. We apply this map to the same functions f_b as before, and similarly as in (6.8) we define the limit of the vector state associated to the ground state $\varphi_N^{(0)}$ of this Hamiltonian. Of course, we first assume that this limit exists. Thus, we need to compute the limit of the expression

$$\langle \varphi_N^{(0)}, S_{1,N}(\sigma_i)\varphi_N^{(0)} \rangle, \quad (i = 1,2,3) \tag{6.95}$$

What do we expect?
It has been shown in the same paper [8] that for $\gamma \in [0,1)$ and $\lambda = -1$, the ground state in the thermodynamical limit is twofold degenerate, still assuming that $0 \leqslant B < 1$.
We will compute the limit of the above expression numerically, and check that this is indeed the case. After this, we show that the ground state of the corresponding classical Hamiltonian lies on the boundary S^2 of B^3, and is given by the points

$$x_\pm = (\pm\sqrt{1 - B^2}, 0, B). \tag{6.96}$$

In fact, these points are precisely obtained as the limits of the corresponding localized eigenstates. To see this, consider the following expression:

$$\langle \frac{\varphi_N^{(0)} \pm \varphi_N^{(1)}}{\sqrt{2}}, S_{1,N}(\sigma_i)\frac{\varphi_N^{(0)} \pm \varphi_N^{(1)}}{\sqrt{2}} \rangle \quad (i = 1,2,3), \tag{6.97}$$

where $\varphi_N^{(1)}$ denotes the first excited state. In contrast to (6.95), the above expression takes the inner product with the localized eigenvectors. The ground state of this Hamiltonian is non-degenerate

for any finite N, and we observe for N up to 5000, that the ground state and the first excited are still not numerical degenerate for the computer. This is in contrast to the Curie-Weiss model. The reason for this probably lies in the fact that the roles of σ_3 and σ_1 are switched in the Curie-Weiss model so that numerical degeneracy can already occur for smaller values of N. We computed the above inner product (6.95) up to $N = 5000$. We did the same for the functions (6.97). Both results are displayed in Figure 6.3 and Figure 6.4.

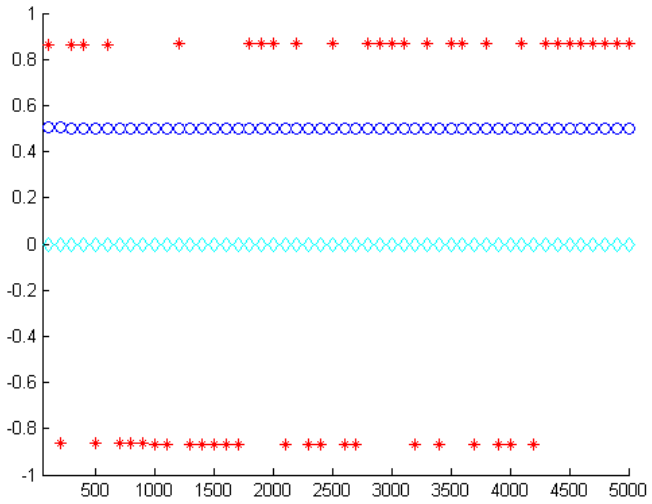

Figure 6.3: The inner product (6.97)*, computed for* $i = 1, 2, 3$*, starting from* $N = 100$ *up to* $N = 5000$*. The blue circles correspond to* $i = 3$*, the red asterisks to* $i = 1$*, and the light blue diamonds to* $i = 2$*. We took* $B = 1/2$*,* $\lambda = -1$ *and* $\gamma = 1/2$ *in the LMG Hamiltonian.*

Similar to the Curie-Weiss Hamiltonian, but now for $i = 1$, the above figure shows that the red asterisks that correspond to $i = 1$ are randomly and equally spread over the numbers $\pm\frac{\sqrt{3}}{2}$. This means that the limiting function is double degenerate. The result should hold for any $\gamma \in [0, 1)$. In the same point of view as for the Curie-Weiss model, we can show that for the functions f_{σ_i} defined by (6.53) up to (6.55), we obtain

$$f_{\sigma_i}((\pm\sqrt{1-B^2}, 0, B)) = \begin{cases} \pm\sqrt{1-B^2}, & \text{if } i = 1; \\ 0. & \text{if } i = 2; \\ B, & \text{if } i = 3. \end{cases} \tag{6.98}$$

Hence the limit of (6.97) corresponds to the points $x_\pm$ and thus to Dirac measures, or, equivalently, to pure states. Keep in mind that these points can only be recovered for the functions f_{σ_i} $(i = 1, 2, 3)$.

Note that the function $\frac{\varphi_N^{(0)} \pm \varphi_N^{(1)}}{\sqrt{2}}$ denotes the localized wave functions, which of course define pure states as well. We have shown numerically that these states converge to pure classical states, exactly as expected and as already known for the double well potential.
In the Curie-Weiss model, we took the ground state eigenvector $\psi_N^{(0)}$. We saw that the ground state was already numerically twofold degenerate for finite N. Due to this degeneracy, the computer already takes the combination $\frac{\psi_N^{(0)} \pm \psi_N^{(1)}}{\sqrt{2}}$ so that we indeed find Dirac measures. These Dirac measures or pure states are identified with the classical limit of these localized wave functions.

If one takes the ground state $\varphi_N^{(0)}$ or the first excited state $\varphi_N^{(1)}$, and computes the limit of (6.95), then we may expect that this limit is defined by the mixed ground state given by

$$\frac{1}{2}(\mu_+ + \mu_-). \tag{6.99}$$

For the numerics, this means that we should find the point $\frac{1}{2}(x_+ + x_-) = (0, 0, B)$, since for this model we do not have numerical degeneracy and therefore no mixing of ground and first excited state. For both the ground state and the first excited state we performed this computation (still for the matrices σ_i) and we recovered precisely the point $(0, 0, B)$, as depicted in Figure 6.4.

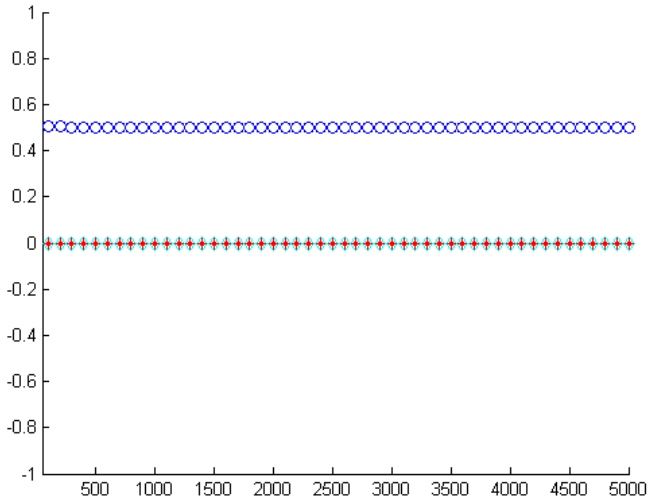

Figure 6.4: The inner product (6.95)*, computed for* $i = 1, 2, 3$*, starting from* $N = 100$ *up to* $N = 5000$ *for both* $\varphi_N^{(0)}$ *and* $\varphi_N^{(1)}$*. The blue circles correspond to* $i = 3$*, the red asterisks to* $i = 1$*, and the light blue diamonds to* $i = 2$*. We took* $B = 1/2$*,* $\lambda = -1$ *and* $\gamma = 1/2$ *in the LMG Hamiltonian.*

Again, this should hold for any $\gamma \in [0, 1)$. We will now show that the corresponding classical (pure) ground state is indeed given by the point in phase space equated by (6.96).

Lemma 6.4. *For* $\gamma \in (0, 1), \lambda = -1$ *and* $B \in [0, 1)$*, the classical LMG-Hamiltonian on the unit ball* B^3 *given by*

$$h_\infty^{LMG}(x, y, z) = -\frac{1}{4}(x^2 + \gamma y^2) - \frac{B}{2}z, \tag{6.100}$$

has a pure doubly degenerate ground state, which is given by

$$x_\pm = (\pm\sqrt{1 - B^2}, 0, B). \tag{6.101}$$

Proof. We apply the method of Lagrange multipliers to these ground states.[8] We set

$$L(x, y, x) = h_\infty^{\mathrm{LMG}}(x, y, z) - \mu(g(x, y, z) - 1). \tag{6.102}$$

[8] According to Definition (2.1) and the explanation in §2.4, the classical ground states are obtained by extremizing the classical LMG-Hamiltonian. According to this definition all extrema are classical ground states. As we know for the classical Curie-Weiss model [22, p.411] and the classical Hamiltonian with double well [22, p.372], this is not true: only minima are considered to be classical ground states. In spirit of these examples, we assume this to be true for the LMG-model as well. We therefore ignore the other extrema and only focus on the minima.

Here, $g(x,y,z) = x^2 + y^2 + z^2$. Taking derivatives of L with respect to x, y, z, μ and setting them equal to zero yields

$$z = -\frac{B}{4\mu}; \tag{6.103}$$

$$y = 0 \quad \text{or} \quad y = -\frac{1}{4}\gamma; \tag{6.104}$$

$$\mu = -\frac{1}{4} \quad \text{or} \quad x = 0; \tag{6.105}$$

$$-(x^2 + y^2 + z^2 - 1) = 0. \tag{6.106}$$

It follows that $\mu = -\frac{1}{4}$, as $\gamma \neq 1$ so that $y = 0$ and then $z = B$. The minimum is obtained for $x \neq 0$ so that $x = \pm\sqrt{1 - B^2}$. □

In the same view as given in the text just below the proof of Lemma 2.5, the $\mathbb{Z}_2$-symmetry is spontaneously broken in this limit. Since the above results hold in particular for $\gamma = 0$, our findings regarding the Curie-Weiss model are explained in this context, since the change of $\sigma_3 \mapsto \sigma_1$ and $\sigma_1 \mapsto \sigma_3$ result in a switch of position 1 and 3 of the vector $x_\pm$. Under this transformation, this shows that the Curie-Weiss model is a particular case of the more general LMG model that includes the parameter γ for non-zero values of γ as well.

Chapter 7

Perturbation in the Curie-Weiss model

In this section we introduce a perturbation in the quantum Curie-Weiss model h_N^{CW} such that the delocalized ground state as displayed in Figure 3.1 localizes already for finite N, but this time it does not do so as a result of numerical degeneracy. We compare the ground state of the perturbed Hamiltonian to the unperturbed one and again make the link with the Schrödinger operator, as explained in Chapter 4. We will see that the perturbation produces a small asymmetric flea on the double well potential corresponding to this Schrödinger operator. The delocalization or collapse of the ground state to the left or the right side of the potential barrier is a result of where exactly this flea is put. We will introduce the notion of explicit symmetry breaking and compare this to the definition of spontaneous symmetry breaking.

7.1 Peturbation in Hamiltonian

Consider again the Hamiltonian for the quantum Curie-Weiss-model:

$$h_N^{\mathrm{CW}} = -\frac{J}{2|\Lambda_N|}\sum_{x,y\in\Lambda_N}\sigma_3(x)\sigma_3(y) - B\sum_{x\in\Lambda_N}\sigma_1(x), \tag{7.1}$$

where Λ_N is an arbitrary finite subset of $\mathbb{Z}$ consisting of N elements, $J > 0$ scales the spin-spin coupling, and B is an external magnetic field. Recall that this local Hamiltonian acts on the Hilbert space $\mathcal{H}_{\Lambda_N} = \otimes_{x\in\Lambda_N} H_x$, where $H_x = \mathbb{C}^2$. We have seen in §3.1 that this Hamiltonian is represented with respect to the standard basis for $\mathcal{H}_{\Lambda_N}$ as the spin Pauli matrices are represented in the standard basis for $\mathbb{C}^2$. We labeled this standard basis consisting of 2^N vectors by β, where $\beta = \{e_{n_1}\otimes e_{n_2}\otimes ...\otimes e_{n_N}\}_{n_1,...,n_N=1}^2$.

These local Hamiltonians define a time evolution on the local algebras $A_{\Lambda_N} = B(\mathcal{H}_{\Lambda_N})$, given by

$$\alpha_t^{(N)}(a_N) = e^{ith_N^{\mathrm{CW}}} a_N e^{-ith_N^{\mathrm{CW}}}. \tag{7.2}$$

We have seen that for each finite N, and each $B \in \mathbb{R}$, this Hamiltonian has a $\mathbb{Z}_2$-symmetry given by 180-degree rotation around the x-axis, locally implemented by the unitary operator $u(x) = \sigma_1(x)$, so that at each $x \in \Lambda_N$ gives $(\sigma_1, \sigma_2, \sigma_3) \to (\sigma_1, -\sigma_2, -\sigma_3)$ since $\sigma_i\sigma_j\sigma_i^* = -\sigma_j$ if $i \neq j$. Hence $u(x)$ sends $\sigma_3(x)$ to $-\sigma_3(x)$, $\sigma_2(x)$ to $-\sigma_2(x)$, but $\sigma_1(x)$ to $\sigma_1(x)$. The $\mathbb{Z}_2$-symmetry was implemented by the unitary operator $u^{(N)}$ on $\mathcal{H}_{\Lambda_N}$ given by

$$u^{(N)} = \otimes_{x\in\Lambda_N}\sigma_1(x). \tag{7.3}$$

It is easy to see that $u^{(N)}$ commutes with the Hamiltonian for every finite N. Therefore, if the ground state eigenvector is non-degenerate, it is an eigenvector of $u^{(N)}$ as well, and therefore its corresponding vector state is $\mathbb{Z}_2$-invariant. We will see this below.
We also remarked that the ensuing $\mathbb{Z}_2$-symmetry on $B(\mathcal{H}_{\Lambda_N})$ is given by the automorphism $\gamma^{(N)}$:

$$\gamma^{(N)}(a) = u^{(N)} a (u^{(N)})^*. \tag{7.4}$$

It follows that we have the local property

$$\alpha_t^{(N)} \circ \gamma_g^{(N)} = \gamma_g^{(N)} \circ \alpha_t^{(N)} \quad (t \in \mathbb{R}, g \in \mathbb{Z}_2 \simeq \{\pm 1\}). \tag{7.5}$$

Thus, in view of Definition 2.3 we have a symmetry of the dynamics. We have shown in §5.3 that for each finite N and $B > 0$ the ground state of the Hamiltonian is unique. For $N = \infty$, and $0 \leqslant B < 1$, the ground state is doubly degenerate and breaks the $\mathbb{Z}_2$-symmetry, as explained in Chapter 6 or in [22, Sec. 10.8].

Transform the ground state eigenvector $\psi_N^{(0)}$ into a vector state by

$$\omega_0^N(a) = \langle \psi_N^{(0)}, a\psi_N^{(0)} \rangle, \quad (a \in A_{\Lambda_N}) \tag{7.6}$$

This state is clearly pure, since $\psi_N^{(0)}$ is a unit vector and $A_{\Lambda_N} = B(\mathcal{H}_{\Lambda_N})$. For $g = 1$ and $g = -1$, it is easy to check that $\omega_0^{(N)} = \omega_0^{(N)} \circ \gamma_g$, since $u^N \psi_N^{(0)} = z\psi_N^{(0)}$ for some $z \in \mathbb{T}$, using $[u^N, h_N^{\mathrm{CW}}] = 0$ and the fact that the ground state is non-degenerate because it is unique. Thus the state ω_0^N is $\mathbb{Z}_2$- invariant. This in combination with (7.5) shows that the $\mathbb{Z}_2$-symmetry is not spontaneously broken in the sense of Definition 2.3.

We are going to define a 'flea'-like perturbation that does not commute with the unitary operator u^N but does commute with the Symmetrizer S. We will give a condition on this flea so that the ground state of the perturbed operator remains unique and therefore lies in the range of S. The perturbation will be defined in a way such that the ground state localizes for finite N, but not as a result of numerical degeneracy. In view of the double well potential displayed in Figure 4.3, we show that this localization can be forced towards the left or right side of the potential barrier, depending on where the flea is put.

Recall from §3.1 that the Symmetrizer S, which is a projection onto the space of all totally symmetric vectors, is given by

$$S(v) = \frac{1}{N!} \sum_{\sigma \in S_n} L_\sigma(v), \tag{7.7}$$

with v is a vector in the N-fold tensor product and L_σ is given by permuting by permuting the factors of v, thus $v_1 \otimes \cdots \otimes v_n \mapsto v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(n)}$. As we have seen, a basis for the space of totally symmetric vectors is given by the vectors $\{|n_+, n_-\rangle|\ n_+ = 0, ..., N\}$, which spans the subspace $\mathrm{Sym}^N(\mathbb{C}^2)$, as mentioned in the beginning of paragraph §3.1.
In order to define a perturbation, again we may pick a basis for $\mathcal{H}_{\Lambda_N}$ and define the perturbation on a basis for $\mathcal{H}_{\Lambda_N}$. Since the original Hamiltonian was defined on the standard basis β, we do the same for the perturbation. In the proof of Theorem 3.1 in §3.1, we have seen there is a bijection between the number of orbits and the dimension of $\mathrm{Sym}^N(\mathbb{C}^2)$. The identification was made as follows:

$$\mathscr{O}^k \leftrightarrow |N-k, k\rangle, \tag{7.8}$$

where k in $|N-k,k\rangle$ labels the number of occurrences of the vector e_2 in any of the basis vectors $\beta_i \in \beta$, and $N-k$ in $|N-k,k\rangle$ labels the occurrence of the vector e_1 in β_i, so that $N-k$ stands for the number of spins in the up direction whilst the second position k denotes the number of down spins. By definition of the Symmetrizer S, any basis vector $\beta_k \in \beta$ in the same orbit $\mathscr{O}^k$ will be mapped under S to the same vector in $\mathrm{Sym}^N(\mathbb{C}^2)$, which equals

$$\frac{1}{\sqrt{\binom{N}{k}}} \sum_{l=1}^{\binom{N}{k}} \beta_{k_l}. \tag{7.9}$$

Here l in β_{k_l} labels the basis vector $\beta_k \in \beta$ within the same orbit $\mathscr{O}^k$. So for each orbit $\mathscr{O}^k$, we have $\binom{N}{k}$ vectors β_k. Hence for each $l = 1, ..., \binom{N}{k}$ the image $S(\beta_{k_l})$ under S, is always the same. It is the coordinate vector written with respect to β. It turns out that the perturbation we are going to define will be very similar to the Symmetrizer operator. Of course, since we have expressed our original Curie-Weiss Hamiltonian with respect to this $|n_+, n_-\rangle$ - basis, we need to do the same for the perturbation we are going to define now.

Since we have a partition of our 2^N-dimensional basis β into $N+1$ orbits, we define a perturbation as follows: we fix $k \in \{0, ..., N\}$ as well as some real number λ_k dependent of k. We denote the perturbation by $V^k_{\lambda_k}$. Then by definition of this perturbation any basis vector β_{k_l} in the corresponding orbit $\mathscr{O}^k$ will be mapped to

$$V^k_{\lambda_k} : \beta_{k_l} \mapsto \lambda_k S(\beta_{k_l}), \qquad \left(l = 1, ..., \binom{N}{k}\right). \tag{7.10}$$

All other $2^N - \binom{N}{k}$ basis vectors β_i will be sent to $S(\beta_i)$. The parameter λ_k is a real number that denotes the strength of the perturbation. When we transform the matrix $[V^k_\lambda]_\beta$ in the β- basis to the matrix written in the $|n_+, n_-\rangle$ - basis, it is obvious that it becomes a diagonal matrix with the value λ_k at entry (k,k).

If we can show that $V^k_{\lambda_k}$ commutes with S and that the ground state eigenvector of the perturbed Hamiltonian $h^{\mathrm{CW}}_N + V^k_{\lambda_k}$ is unique, then we may conclude that the ground state lies in the subspace $\mathrm{Sym}^N(\mathbb{C}^2)$. The reason for this is the same as for the unperturbed Curie-Weiss Hamiltonian: proving these properties makes that this eigenvector lies in the $\mathrm{ran}(S) = \mathrm{Sym}^N(\mathbb{C}^2)$, so that we may diagonalize this Hamiltonian represented as a matrix that can be written with respect to the symmetric subspace, which will be a tridiagonal matrix of dimension $N+1$ as well. This makes computations much easier, and we can compare both systems, i.e. the unperturbed one and the perturbed one. Similarly as for the Curie-Weiss model, a sufficient condition for uniqueness of the ground state of the perturbed matrix, originally written with respect to the standard basis for $\mathcal{H}_{\Lambda_N}$, is non-negativity and irreducibility, so that we can apply Lemma 5.12 and Theorem 5.11. This depends, of course, on the parameter λ_k. We will come back to this later.

In order to show that the commutator relation is zero, i.e., $[S, V^k_\lambda] = 0$, it suffices to show this for a basis. We check it for the standard basis β of the N-fold tensor product. Fix a basis vector β_j in $\mathscr{O}^k$. If we take any basis vector β_i not in $\mathscr{O}^k$, then by definition

$$V^k_\lambda(\beta_i) = S(\beta_i). \tag{7.11}$$

If we take any vector β_i in the orbit $\mathscr{O}^k$, then

$$\begin{aligned} V_\lambda^k S(\beta_i) &= V_\lambda^k \frac{1}{\sqrt{\binom{N}{k}}} \sum_{l=1}^{\binom{N}{k}} \beta_l \\ &= \frac{1}{\sqrt{\binom{N}{k}}} \sum_{l=1}^{\binom{N}{k}} V_\lambda^k(\beta_l) \\ &= \frac{\lambda}{\sqrt{\binom{N}{k}}} \sum_{l=1}^{\binom{N}{k}} S(\beta_l) \\ &= \lambda S^2(\beta_i) \\ &= \lambda S(\beta_i). \end{aligned} \tag{7.12}$$

since $S(\beta_i)$ lies in the orbit $\mathscr{O}^k$ and thus is a linear combination of all other $\binom{N}{k}$ vectors in this orbit.

On the other hand, if we take any basis vector β_i not in $\mathscr{O}^k$, then again as before,

$$SV_\lambda^k(\beta_i) = S^2(\beta_i) = S(\beta_i) \tag{7.13}$$

since V_λ^k acts as the Symmetrizer on vectors in $\mathrm{ran}(S) = \mathrm{Sym}^N(\mathbb{C}^2)$ that are not equal to β_j. If we take any vector β_i in $\mathscr{O}^k$ then,

$$SV_\lambda^k(\beta_i) = S\lambda S(\beta_i) = \lambda S(\beta_i). \tag{7.14}$$

We see that for all basis vectors $\beta_i \in \beta$ we have $[S, V_\lambda^k](\beta_i) = 0$.

The last step is to show that the Hamiltonian $-(h_N^{\mathrm{CW}} + V_\lambda^k)$, written with respect to the standard basis β for $\mathcal{H}_{\Lambda_N}$, is a non-negative and irreducible matrix. Since the off-diagonal elements are completely determined by the unperturbed Hamiltonian and are never zero, the matrix can never be decomposed into two blocks, so that it remains irreducible. Non-negativity is achieved when

$$\frac{J}{2N}(2n_+ - N)^2 - \lambda_{n_+} \geqslant 0. \tag{7.15}$$

This depends of course on $k = n_+$ and hence on the orbit $\mathscr{O}^{n_+}$ where we have put the perturbation. Any $V_{\lambda_{n_+}}^{n_+}$ satisfying this inequality guarantees non-negativity. If we assume that this is satisfied, then together with the fact that $h_N^{\mathrm{CW}} + V_{\lambda_{n_+}}^k$ commutes with S, we can conclude in the same spirit as §5.3 that the ground state of the perturbed Hamiltonian is unique, and therefore indeed lies in $\mathrm{ran}(S) = \mathrm{Sym}^N(\mathbb{C}^2)$. Finally, knowing now that we may diagonalize the perturbed Hamiltonian with respect to the symmetric basis $|n_+, n_-\rangle$, we use the fact that the sum of two linear transformations written with respect to a basis individually equals the sum of both linear transformations if this total sum is written with respect to the basis, i.e.:

$$[h_N^{\mathrm{CW}}]_{|n_+,n_-\rangle} + [V_{\lambda_k}^k]_{|n_+,n_-\rangle} = [h_N^{\mathrm{CW}} + V_{\lambda_k}^k]_{|n_+,n_-\rangle}. \tag{7.16}$$

Therefore, since we may diagonalize $h_N^{\mathrm{CW}} + V_{\lambda_k}^k$ in the symmetric basis $|n_+, n_-\rangle$, the above observation (7.16) ensures that it suffices to diagonalize the sum of the individual matrices represented in this basis, i.e., the tridiagonal matrix $[h_N^{\mathrm{CW}}]_{|n_+,n_-\rangle}$ (viz. (3.1)) and the perturbation matrix $[V_{\lambda_k}^k]_{|n_+,n_-\rangle}$.

Recall that in §3.2 the ground state $\psi_N^{(0)}$ of the unperturbed Hamiltonian h_N^{CW} was approximately given by two Gaussians (for N large), each of them located in one of the wells of the potential, and was given by

$$\psi_N^{(0)} \cong \frac{T_a(\varphi_0) + T_{-a}(\varphi_0)}{\sqrt{2}}. \tag{7.17}$$

In fact, this is true for any finite N, since the ground state is unique, as we have proven in §5.3. However, due to numerical degeneracy of the ground state and the first excited state for about $N \geqslant 80$, these two states will form a linear combination $\chi_\pm$ given by (3.29). By a simple calculation, we found that for these relative large values of N, the (numerical) degenerate ground state is given by

$$\chi_\pm \cong T_{\pm a}(\varphi_0), \tag{7.18}$$

where the functions $\varphi_0(x)$ have to be understood as functions on a discrete grid. For $N < 80$, we observed that a plot of the ground state displayed a doubly peaked Gaussian, as expected from (7.17). This made sense, since the energy levels in the latter case are not degenerate, not even for the computer.

As we have mentioned we wanted to show that, due to the perturbation, the (unique) ground state localizes for finite N. We have just argued that this happens already for $N \geqslant 80$, but this was a result of numerical inaccuracy/degeneracy. The question is then if our perturbation forces the ground state to localize for finite N in such a way that it will be not a result of numerical degeneracy. The answer is yes. It depends on the parameter λ_{n_+} with n_+ denoting the n_+^{th}- position in the diagonal matrix of the perturbation. Completely analogously as in Chapter 4, we can extract the potential corresponding to the perturbed Hamiltonian $h_N^{\mathrm{CW}} + V^k_{\lambda_{n_+}}$, written with respect to the symmetric base. We scaled this Hamiltonian by $1/N$ and translated the potential so that its minima are set to zero. We have made a plot of this potential (Figure 7.1). For convenience, we scaled the domain to the unit interval. Moreover, we plotted the ground state of this Hamiltonian and the one corresponding to the unperturbed one (Figure 7.2). We observe a localization of the ground state in the right sided well. Simulations showed that the eigenvalues of the perturbed Hamiltonian are non-degenerate, so that the ground state is indeed unique, also for the computer. Hence, the localization is not a result of numerical degeneracy. We did a similar simulation for the flea but now located on the right site of the barrier (Figure 7.3). We see a localization of the ground state to the left side of the barrier (Figure 7.4).

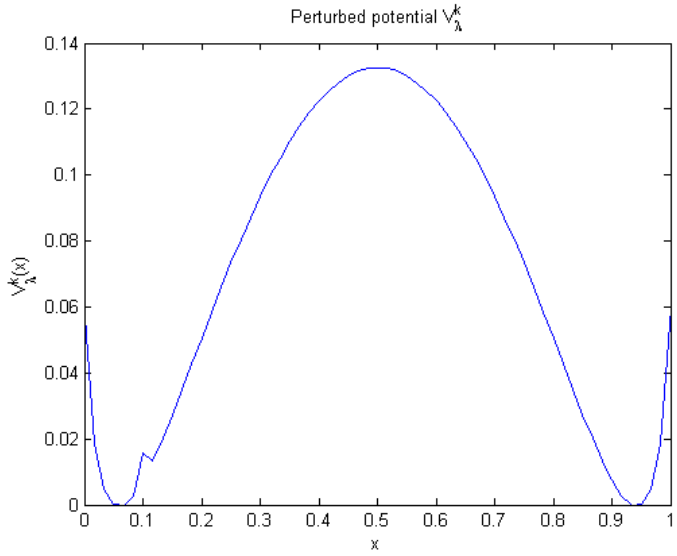

Figure 7.1: The perturbed potential energy computed from the tridiagonal matrix $h_N^{CW} + V_{\lambda_k}^k$ *for* $N = 60$, $\lambda_k = 0.5$, $k = 7$, $J = 1$ *and* $B = 1/2$. *This potential has a 'flea' on the left side of well due the perturbation* $V_{\lambda_k}^k$.

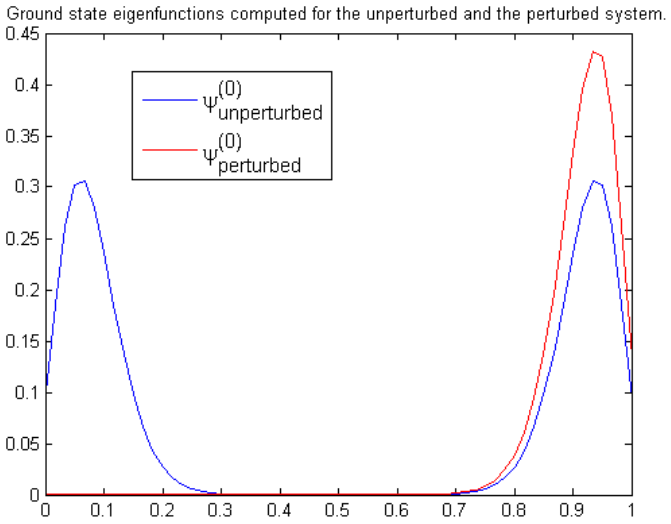

Figure 7.2: The corresponding ground state (in red) of the perturbed Hamiltonian $h_N^{CW} + V_{\lambda_k}^k$ *is already localized for* $N = 60$, $\lambda_k = 0.5$, $k = 7$, $J = 1$ *and* $B = 1/2$. *For these values of* λ_k *and* k, *still condition* (7.15) *is satisfied. The localization takes place on the right side of the well, since the flea lifts the potential on the left side.*

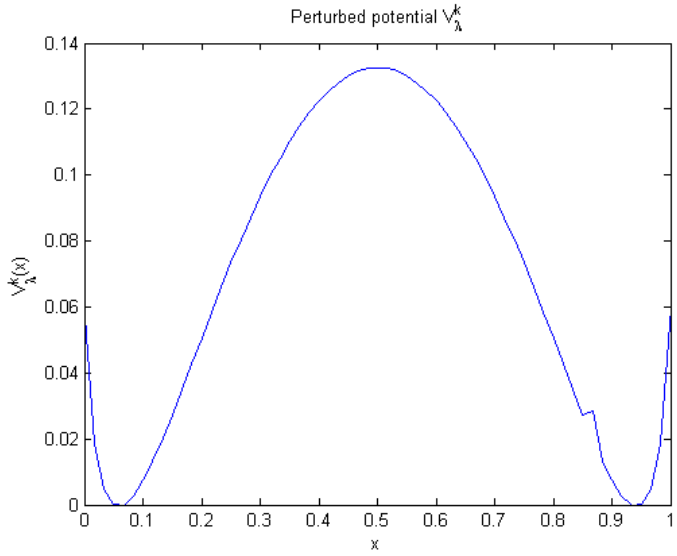

Figure 7.3: The perturbed potential energy computed from the tridiagonal matrix $h_N^{CW} + V_{\lambda_k}^k$ for $N = 60$, $\lambda_k = 0.5$, $k = 7$, $J = 1$ and $B = 1/2$. This potential has a 'flea' on the right side of the well due the perturbation $V_{\lambda_k}^k$.

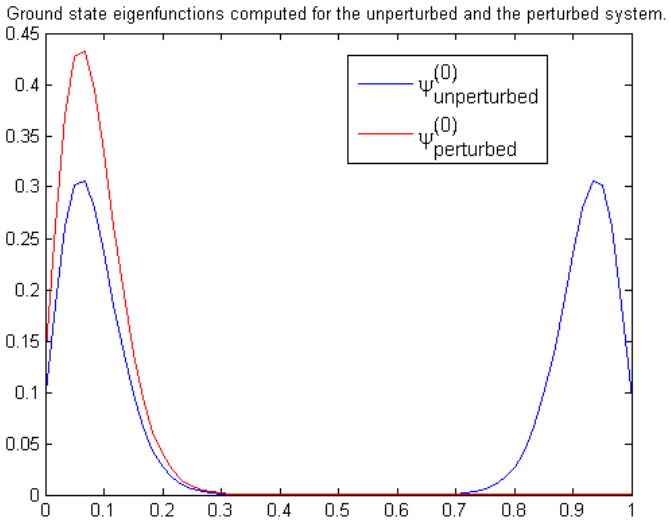

Figure 7.4: The corresponding ground state (in red) of the perturbed Hamiltonian $h_N^{CW} + V_\lambda^k$ is already localized for $N = 60$, $\lambda_k = 0.5$, $k = N - 7$, $J = 1$ and $B = 1/2$. For these values of λ_k and k, condition (7.15) is still satisfied. Localization takes place on the left side of the barrier, since the flea lifts the potential on the right side.

Our conclusion is that due to this 'flea'-like perturbation, the ground state will localize in one of the wells depending on where the flea is put. This localization may be understood from energetic considerations. For example, if $\lambda_{n_+} > 0$ such that condition (7.15) is satisfied and the perturbation is located on the right, then the relative energy in the left-hand part of the double well is lowered, so that localization will be to the left. This result matches exactly the work done in [34], where the Schrödinger operator with a symmetric double well was studied rather than quantum spin systems.

The last topic of this section is to relate these results to symmetry breaking. Given the

perturbed Hamiltonian $h_N^{\mathrm{CW}} + V_{\lambda_k}^k$ such that (7.15) is satisfied, we know that the unique ground state lies in $\mathrm{Ran}(S) = \mathrm{Sym}^N(\mathbb{C}^2)$. However, we do not have a $\mathbb{Z}_2$-symmetry of the system since this perturbed Hamiltonian does not commute with the unitary operator $u^{(N)} = \otimes_{x=1}^N \sigma_1(x)$ implementing this $\mathbb{Z}_2$-symmetry:

Lemma 7.1. *The unitary operator $u^{(N)} = \otimes_{x=1}^N \sigma_1(x)$ does not commute with $V_{\lambda_k}^k$, and therefore the ground state of the perturbed Hamiltonian $h_N^{CW} + V_\lambda^k$ is not $\mathbb{Z}_2$-invariant.*

Proof. It is easy to see that $u^{(N)}$ maps any vector in the orbit $\mathscr{O}^k$ to vectors in $\mathscr{O}^{N-k}$: fix a basis vector $\beta_{k_l} \in \mathscr{O}^k$, ($k = 0, ..., N$ and $l = 1, ..., \binom{N}{k}$). Then

$$\begin{aligned} &V_{\lambda_k}^k \beta_{k_l} = \lambda_k S(\beta_{k_l}); \\ &u^{(N)}(\beta_{k_l}) = \sigma_1(e_{n_1}) \otimes \cdots \otimes \sigma_1(e_{n_N}). \end{aligned} \tag{7.19}$$

Here, $e_{n_i} = \binom{1}{0}$ or $\binom{0}{1}$. Since $\beta_{k_l} \in \mathscr{O}^k$, then by definition of the σ_1, we have $u^{(N)}(\beta_{k_l}) \in \mathscr{O}^{N-k}$.

Now compute:

$$(u^{(N)} V_{\lambda_k}^k)(\beta_{k_l}) = (u^{(N)} V_{\lambda_k}^k)(e_{n_1} \otimes \cdots \otimes e_{n_N}) = \lambda_k S(\sigma(e_{n_1}) \otimes \cdots \otimes \sigma(e_{n_N})). \tag{7.20}$$

On the other hand:

$$(V_{\lambda_k}^k u^{(N)})(\beta_{k_l}) = (V_{\lambda_k}^k u^{(N)})(e_{n_1} \otimes \cdots \otimes e_{n_N}) = \lambda_{N-k} S(\sigma(e_{n_1}) \otimes \cdots \otimes \sigma(e_{n_N})). \tag{7.21}$$

Hence, as soon as $\lambda_{N-k} \neq \lambda_k$, the above two equations are not equal, so that $V_{\lambda_k}^k$ does not commute with $u^{(N)}$. But this is satisfied, since $\lambda_{N-k} = 1$ and $\lambda_k \neq 1$.

We will now prove the last assertion by contradiction. Denote $\tilde{\psi}_N^{(0)}$ to be the (unique) ground state eigenvector of $h_N^{\mathrm{CW}} + V_{\lambda_k}^k$. Transform it into a (pure vector) state:

$$\tilde{\omega}_N^{(0)}(a) = \langle \tilde{\psi}_N^{(0)}, a\tilde{\psi}_N^{(0)} \rangle. \tag{7.22}$$

Assume this state is $\mathbb{Z}_2$-invariant. Then, in particular for the non-trivial element $\gamma = -1 \in \mathbb{Z}_2$, we have

$$\tilde{\omega}_N^{(0)}(\gamma_{-1}(a)) = \langle (u^{(N)})^* \tilde{\psi}_N^{(0)}, a(u^{(N)})^* \tilde{\psi}_N^{(0)} \rangle = \langle \tilde{\psi}_N^{(0)}, a\tilde{\psi}_N^{(0)} \rangle. \tag{7.23}$$

By uniqueness of the ground state, this would imply that $u^{(N)}\psi_N^{(0)} = z\psi_N^{(0)}$ for some z with $|z| = 1$, and hence also that $[h_N^{\mathrm{CW}} + V_{\lambda_k}^k, u^{(N)}] = 0$, which is a contradiction with the first part of the proof. Therefore, the ground state of the perturbed Hamiltonian is not $\mathbb{Z}_2$-invariant. This completes the proof the lemma. □

From this lemma, it follows also that there is no symmetry of the dynamics in the sense of Definition 2.3. Therefore, we cannot speak about spontaneous symmetry breaking of the ground state. Since the perturbation forces the ground state to localize in one of the wells, in the classical limit the ground state will be a pure state. This is in contrast to the case without perturbation: in theory the (doubly peaked) ground state will converge to a mixed ground state if $N \to \infty$[1]. We call this phenomena explicit symmetry breaking meaning that due to a small perturbation of the Hamiltonian, the ground state will localize already for finite N, with a pure state being its classical limit. The direction of localization to either the left or the right side of the potential barrier can be controlled by the perturbation.

[1]Keep still in mind that the unperturbed Hamiltonian does not give this result, since the eigenvectors already mix due to the numerical degeneracy of the computer. Therefore, the classical limit is pure as well.

When one considers the Schrödinger operator with a double well potential, symmetric around $x = 1/2$, and defined on the Hilbert space $L^2([0,1])$, the ensuing $\mathbb{Z}_2$ symmetry is given by reflection around $x = 1/2$ given by $\tau_{1/2}(f)(x) := f(1-x)$. If one adds an asymmetric flea on the potential as displayed in the figure above, then it is clear that the Schrödinger Hamiltonian does not commute anymore with $\tau_{1/2}$, so that completely analogously to the above observation, we do not have a symmetry of the dynamics and hence no SSB, even though the ground state still remains unique, because the uniqueness theorems in §5.4 remain applicable to the potential. It has been shown in [34] that the ground state localized exactly a same way as we just have shown. Therefore, our findings concerning the (explicit) symmetry breaking of the ground state of the Curie-Weiss model completely match the Schrödinger operator analog.

Remark.
We have seen the the ground state of the unperturbed Curie-Weiss model has a classical limit as a state on $C(B^3)$. This should be a mixed state, like for the LMG-model. However, we have seen that due to numerical degeneracy of the ground state, the ground state eigenvector localizes already for finite $N \geqslant 80$, so that the classical limit is a pure state. This 'numerical symmetry breaking' therefore has the same effect as explicit symmetry breaking for the perturbed Hamiltonian. The disadvantage is that we cannot take N too big (like $N = 5000$) in order to check that we have a mixed classical limit, as expected from [22, Sec. 10.1].

Chapter 8

Discussion and further research

Let us summarize our findings and see what can be said regarding spontaneous symmetry breaking of quantum spin systems and their classical limits. Although the only spin system we have studied in detail was the quantum Curie-Weiss model, we can conclude some important results. Probably the most important result is the link we have made between the quantum Curie-Weiss Hamiltonian and a Schrödinger operator with a symmetric double well potential. We have shown that the scaled quantum Curie-Weiss Hamiltonian restricted to the symmetric subspace $\mathrm{Sym}^N(\mathbb{C}^2)$ was an approximation of a discretization of a Schrödinger operator with a symmetric double well potential, defined on $L^2([0,1])$. Using the fact that this Schrödinger operator has a classical limit with corresponding ground state given by Dirac measures, we might conclude the same for the spin system. We have also seen in Chapter 6 that the ground state of the quantum spin Hamiltonian has another classical limit, this time defined on $C(B^3)$. Both limiting cases have in common that the ground state is doubly-degenerate and breaks the $\mathbb{Z}_2$-symmetry spontaneously, at least in the regime $0 \leqslant B < 1$. Subsequently, we showed in Chapter 7 that due to a small perturbation this $\mathbb{Z}_2$-symmetry can already be explicitly broken for finite N, resulting in a *pure* ground state in the classical limit. This form of *explicit* symmetry breaking due to a small perturbation has also been studied from a similar perspective for the Schrödinger operator with a symmetric double well potential [22], [34]. We have seen that this was completely in accordance with our findings regarding the quantum Curie-Weiss model.

We started this thesis by mentioning the concept of *asymptotic emergence*. We saw that the natural phenomenon spontaneous symmetry breaking (SSB) is an example of what we called an *emergent* feature. We considered the pair (H_1, L_1), with H_1 classical mechanics on $C(B^3)$, and L_1 the quantum Curie-Weiss spin chain on a finite line. Another example for which SSB is an emergent feature is the pair (H_2, L_2), with H_2 quantum mechanics on $B_0(L^2(\mathbb{R}))$ and L_2 classical mechanics of a particle on a subset of the real line. In fact, based on the connection between the pertinent Schrödinger operator and the quantum Curie-Weiss model, these pairs are related. There should be more research to get a better understanding about this relation, since our findings are partly based on numerical simulations. For example, we were not able to prove mathematically that the ground state eigenfunction of the compressed Curie-Weiss Hamiltonian localizes on a subset of order $\sqrt{N}$. Apart from that, another important omission is that we do not know if the excited states of the Curie-Weiss Hamiltonian defined on $\bigotimes_{n=1}^{N} \mathbb{C}^2$ are in the symmetric subspace or not. We only know this for the ground state. Therefore, considering the tridiagonal matrix, we may not a priori conclude that for example the first excited state of this matrix corresponds also to the first excited state of the original Curie-Weiss Hamiltonian. As a result, when passing to the classical limit from the (scaled) tridiagonal matrix, we should beware of convergence of the first excited state. However, numerical results have shown that the desired classical limit, starting from the quantum ground and first excited state, was in fact obtained. In view of the

pair (H_1, L_1), we defined a deformation quantization. Although this map was only defined for some class of functions, not for all functions on $C(B^3)$, this definition was sufficient to pass to the classical ground states. It is still not so clear how to define this map on the whole algebra $C(B^3)$. Moreover, in view of Theorem E.5 the construction of this map is not unique, i.e., different choices can lead to quasi-symmetric sequences which converge to the desired limit. In addition, the proof of weak*-convergence of the reduced density matrices involved was partly based on numerical simulations, since we were not able to give an explicit expression for the ground state eigenvector.

More research is needed to understand better the connection between such pairs (H, L). We have mentioned some interesting topics regarding this relation in the beginning of this thesis. For example, it is not so clear how to construct a classical Hamiltonian corresponding to H from the underlying quantum Hamiltonian belonging to L. A useful theorem that connects at least the classical dynamics to quantum dynamics for spin systems can be found in [22, Thm. 10.22] and [22, Cor. 10.23]. We have seen in the introduction of this thesis that the quantum Ising model has both a classical and a quantum limit. Both (different) limits have a doubly-degenerate ground state that displays SSB, like for the classical Curie-Weiss model. This non-trivial result is definitely a very interesting topic for further research. However, the disadvantage of the quantum Ising model is that its Hamiltonian represented with respect to the canonical basis for $\bigotimes_{n=1}^{N} \mathbb{C}^2$ has alternating positive and negative entries so that the Perron-Frobenius theorem cannot be applied to this matrix, and hence uniqueness of the ground state does not follow easily, like for the Curie-Weiss model. Moreover, this model takes only nearest neighbour interactions so that it does not commute with the Symmetrizer operator. Thus, in order to compute the ground state, we cannot restrict ourselves to this subspace and numerical simulations seem pretty hopeless. Inspired by the connection between the quantum Curie-Weiss Hamiltonian and the Schrödinger operator with a symmetric potential, the general question is if there are more quantum spin systems that can be related to Schrödinger operators with some potential. Like for the quantum-Curie-Weiss model, the crucial property is the existence of a subspace of $\bigotimes_{n=1}^{N} \mathbb{C}^2$ and a basis such that the spin Hamiltonian, written with respect to this basis of the subspace, is a tridiagonal matrix. It is a priori not clear if such a subspace also exists for other quantum spin Hamiltonians. A complete new research project relating quantum spin systems to Schrödinger operators can therefore be launched.

In short, lots of interesting topics regarding asymptotic emergence are still not well understood and can therefore be the subject for new research.

Appendix A

C^*-algebras

C^*-algebras play a central role in modeling the quantum (and even the classical) systems in which we are interested. Therefore, we outline some basic concepts related to C^*-algebras that can be found in [28], [29]. We begin with some definitions.

Definition A.1. *An involution on an algebra A is a conjugate-linear map $a \mapsto a^*$ on A, such that $a^{**} = a$ and $(ab)^* = b^*a^*$ for all $a, b \in A$. The pair $(A, *)$ is called a $*$-algebra.*

Definition A.2. *A homomorphism from an algebra A to an algebra B is a linear map $\varphi : A \to B$ such that $\varphi(ab)\varphi(a)\varphi(b)$ for all $a, b \in A$. If $\varphi : A \to B$ is a homomorphism of $*$-algebras A and B, and φ preserves adjoints, that is $\varphi(a^*) = \varphi(a)^*$ $(a \in A)$, then φ is called a $* - homomorphism$. If in addition φ is a bijection, then it is a $* - isomorphism$. An automorphism of a $*$-algebra A is a $*$-isomorphism $\varphi : A \to A$. The set of all automorhpisms of A is denoted by $Aut(A)$. This set forms a group under composition. If A is unital and u is unitary in A, then*

$$a \mapsto uau^* \quad (a \in A), \tag{A.1}$$

is an automorphism of A. Such an automorphism, given by conjugation with a unitary, is called inner. In general, not every automorphism of a C^*-algebra is inner (except,for example when $A = B(H)$).

Definition A.3. *A $Banach\ * - algebra$ is a $*$-algebra A together with a complete submultiplicative norm (i.e., $||ab|| \leqslant ||a|| \cdot ||b||$) such that $||a||^* = ||a||$ $(a \in A)$. If, in addition, A has a unit such that $||1|| = 1$, we call A a $unital\ Banach\ * - algebra$. A C^*-algebra is a Banach $*$-algebra such that*

$$||a^*a|| = ||a||^2 \quad (a \in A). \tag{A.2}$$

Now, we introduce the concept of the dynamics of a physical system. They describe how observables (i.e., elements of the C^*-algebra) evolve over time. A natural approach is to look at the time evolution of the observables, $t \mapsto a(t)$. This is called the Heisenberg picture. The time evolution induces a one-parameter subgroup of automorphisms $t \mapsto \alpha_t$ of the observable algebra.

Definition A.4. *The dynamics of a C^*-algebra A is given by a continuous homomorphism*

$$\alpha : \mathbb{R} \to Aut(A); \tag{A.3}$$

$$t \mapsto \alpha_t, \tag{A.4}$$

where we use the notation $\alpha_t \equiv \alpha(t)$. Continuity here means strong continuity, in that for each $a \in A$, the map $t \mapsto \alpha_t(a)$ from $\mathbb{R}$ to A is continuous (so that the map $\mathbb{R} \times A \to A$ given by $(t, a) \mapsto \alpha_t(a)$ is continuous, as usual for group actions).

To make the connection between the abstract C^*-algebraic picture and the physical world, it is necessary to have a way to describe expectation values of measurement outcomes. This naturally leads to the notion of a *state* on a C^*-algebra. Using such states there is then a canonical way, the *GNS construction*, to represent the system on a Hilbert space.

Definition A.5. *A linear map $\varphi : A \to B$ between two C^*-algebras A and B is said to be positive if $\varphi(A^+) \subset \varphi(B^+)$. Here, A^+ and B^+ denote the sets of self-adjoint elements with positive spectrum.*

Definition A.6. *A state $\omega : A \to \mathbb{C}$ is a positive linear functional of norm 1. We denote by $S(A)$ the set of states of A.*

Definition A.7. *Let A be a C^*-algebra and $\mathcal{H}$ be a Hilbert space. A representation of A on $\mathcal{H}$ is a $*$-homomorphism $\pi : A \to B(\mathcal{H})$.*

it is a basic result that for representations π of C^*-algebras, one automatically has $||\pi(a)|| \leqslant ||a||$ for all $a \in A$. It follows that the representation is automatically continuous with respect to the norm topology.

Definition A.8. *A representation $\pi : A \to B(\mathcal{H})$ is called $non-degenerate$ if the set $\pi(A)\mathcal{H}$ is dense in $\mathcal{H}$. It is called cyclic if there exists some vector $\Omega \in \mathcal{H}$ such that $\pi(A)\Omega$ is a dense subset of $\mathcal{H}$. Such an Ω is called a cyclic vector.*

We are now in the position to state the *GNS construction*, named after Gel'fand, Naimark and Segal.

With each positive linear functional, there is an associated representation. Suppose that ω is a positive linear functional on a C^*-algebra A. Define the set

$$N_\omega = \{a \in A |\ \omega(a^*a) = 0\}. \tag{A.5}$$

It is not difficult to see that N_ω is a closed left ideal of A. We can therefore form the quotient vector space $H_\omega = A/N_\omega$ and write $[a]$ for the equivalence class of $a \in A$ in this quotient. This means that $[a] = [b]$ if and only if $a = b + n_0$ for some $n_0 \in N_\omega$. We can define a map on $H_\omega \times H_\omega$:

$$H_\omega \times H_\omega \to \mathbb{C}; \tag{A.6}$$

$$(a + N_\omega, b + N_\omega) \mapsto \omega(a^*b). \tag{A.7}$$

It can be shown that this map is a well-defined inner product on H_ω. By taking the completion with respect to this inner product we obtain the Hilbert space $\mathcal{H}_\omega$.
Next we define the representation π_ω by defining the action of $\pi_\omega(A)$ on the dense subset H_ω of $\mathcal{H}_\omega$. Let $[b] \in H_\omega$, then we define

$$\pi_\omega : A \to B(H_\omega) \tag{A.8}$$

$$\pi_\omega(a)[b] = [ab]. \tag{A.9}$$

It is easy to check that this is well-defined. Moreover, we have

$$||\pi_\omega(a)[b]||^2 \leqslant \langle [ab], [ab] \rangle = \omega(b^*a^*ab) \leqslant ||a||^2 \omega(b^*b) = ||a||^2 \cdot ||[b]||_{H_\omega}, \tag{A.10}$$

where $||\cdot||$is the norm on the C^*-algebra. Therefore, $\pi_\omega(a)$ is bounded on a dense subset of $\mathcal{H}_\omega$. It is not difficult to check that π_ω is linear on this dense subset, hence it can be uniquely extended to a bounded operator on $\mathcal{H}_\omega$, which we again denote by π_ω. From the definition of π_ω, it is easy to check that this map is a $*$-homomorphism.[1] If we define $\Omega_\omega = [I]$, it is clear that Ω_ω is cyclic for π_ω. Moreover, for each $a \in A$:

$$\langle \Omega_\omega, \pi_\omega(a)\Omega_\omega \rangle = \langle [I], [a] \rangle = \omega(a). \tag{A.11}$$

[1] If necessary, we add a unit I to A, or we take an approximate identity $\{e_\lambda\}$ for A. In the latter case, it is easy to show that the equivalence class of the net $\{e_\lambda\}$ converges to some cyclic unit vector in H_ω.

If ω is a state, then it can be shown that Ω_ω has norm 1, and is therefore a cyclic unit vector.

This brings us to the first theorem.

Theorem A.9. *Let A be a C^*-algebra and ω a state on A. Then there exists a triple $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$, where $\mathcal{H}_\omega$ is a Hilbert space and π_ω a representation of A on $\mathcal{H}_\omega$, such that Ω_ω is a cyclic unit vector for π_ω, and in addition we have*

$$\omega(a) = \langle \Omega_\omega, \pi_\omega(a)\Omega_\omega \rangle \quad (a \in A). \tag{A.12}$$

This triple is unique in the sense that if $(\pi, \mathcal{H}, \Psi)$ is another such triple, there is a unitary $U : \mathcal{H}_\omega \to \mathcal{H}$ such that $U\Omega = \Psi$ and $\pi(a) = U\pi_\omega(a)U^*$ for all $a \in A$.

Proof. The first part of the theorem is given above. It remains to be shown that the construction is essentially unique. Suppose that $(\pi, \mathcal{H}, \Psi)$ is another such triple. Define $U : \mathcal{H}_\omega \to \mathcal{H}$ by setting

$$U\pi_\omega(a)\Omega_\omega = \pi(a)\Psi \quad (a \in A). \tag{A.13}$$

This is a linear map of a dense subspace of $\mathcal{H}_\omega$ onto a dense subspace of $\mathcal{H}$, using that Ψ is cyclic by assumption. Moreover, for each $a, b \in A$ we have

$$\langle U\pi_\omega(a)\Omega_\omega, U\pi_\omega(b)\Omega_\omega \rangle = \langle \pi(a)\Psi, \pi(b)\Psi \rangle = \omega(a^*b) = \langle \pi_\omega(a)\Omega_\omega, \pi_\omega(b)\Omega_\omega \rangle. \tag{A.14}$$

This shows that U is well defined as well as isometric, so that it extends to $\mathcal{H}_\omega$ by continuity. It then follows that its image is the closure of $\pi(A)\Psi$, which is $\mathcal{H}$. Thus U is surjective and hence unitary. Moreover, we compute

$$U\pi_\omega(a)\pi_\omega(b)\Omega = U\pi_\omega(ab)\Omega = \pi(ab)\Psi = \pi(a)\pi(b)\Psi = \pi(a)U\pi_\omega(b)\Omega. \tag{A.15}$$

We conclude that $U\pi_\omega(a) = \pi(a)U \ \ (a \in A)$ on the dense space $\pi_\omega(A)\Omega_\omega$, and hence everywhere. □

Note that automorphisms preserve all the algebraic relations of the algebra. Hence they are a natural tool to model symmetries. There is an important corollary that follows from the uniqueness of the GNS representation. If α is an automorphism of A and ω is invariant under the action of this automorphism (e.g., a ground state of a physical system is invariant under some symmetry), then α is implemented by a unitary in the GNS representation. The precise statement is as follows:

Theorem A.10. *Let A be a C^*-algebra and α an automorphism of A. Suppose that ω is a state on A such that $\omega \circ \alpha = \omega$. then there is a cyclic representation $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$ such that*

$$\omega(a) = \langle \Omega_\omega, \pi_\omega(a)\Omega_\omega \rangle, \tag{A.16}$$

and a unitary $U \in B(\mathcal{H}_\omega)$ such that $\pi_\omega \circ \alpha(a) = U\pi_\omega(a)U^*$ and $U\Omega_\omega = \Omega_\omega$.

Proof. Let $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$ be the GNS representation for the state ω. Note that $(\pi_\omega \circ \alpha, \mathcal{H}_\omega, \Omega_\omega)$ is another GNS triple:

$$\langle \Omega_\omega, \pi_\omega(\alpha(a))\Omega_\omega \rangle = \omega(\alpha(a)) = \omega(a) \quad (a \in A). \tag{A.17}$$

Moreover, Ω_ω is again cyclic since α is an automorphism. By uniqueness of the GNS triple (Theorem A.9), there is a unitary operator U such that $\pi_\omega \circ \alpha(a) = U\pi_{\omega(a)}U^*$. This U is defined by

$$U\pi_\omega(a)\Omega_\omega = \pi_\omega(\alpha(a))\Omega_\omega. \tag{A.18}$$

This definition is well-defined. To see this, denote $[a] = \pi_\omega(a)\Omega_\omega$ and $[a'] = \pi_\omega(a')\Omega_\omega$, both elements of H_ω. If $[a] \sim [a']$, then $a = a' + N_\omega$, so that $a - a' \in N_\omega$. It follows that

$$\pi_\omega(\alpha(a))\Omega_\omega - \pi_\omega(\alpha(a'))\Omega_\omega = [\alpha(a - a')I]. \tag{A.19}$$

We have to prove that

$$\pi_\omega(\alpha(a))\Omega_\omega = \pi_\omega(\alpha(a'))\Omega_\omega. \tag{A.20}$$

Hereto, we show that (A.19) is zero, by proving that $\alpha(a - a') \in N_\omega$. We compute

$$\omega(\alpha(a - a')^*\alpha(a - a')) = \omega(\alpha(a - a')^*(a - a')) = \omega(a - a')^*(a - a') = 0, \tag{A.21}$$

using that α is a automorphism, the invariance of ω under α and that $a - a' \in N_\omega$. By definition of ω, we have

$$0 = ||[\alpha(a - a')I]||^2, \tag{A.22}$$

which implies immediately that

$$[\alpha(a - a')I] = 0. \tag{A.23}$$

We conclude that

$$\pi_\omega(\alpha(a))\Omega_\omega = \pi_\omega(\alpha(a'))\Omega_\omega. \tag{A.24}$$

Therefore, U is well-defined and this is exactly the unitary we were looking for. □

Appendix B

Discretization

This information provided in this appendix is based on [21] and [19]. These results have been used in §4.5.

Recall from calculus that the following approximations are valid for the derivative of single-variable functions $f(x)$. The first one is called the forward difference approximation and is an expression of the form

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h) \quad (h > 0). \tag{B.1}$$

The backward difference approximation is of the form

$$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h) \quad (h > 0). \tag{B.2}$$

Furthermore, the central difference approximation is

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2) \quad (h > 0). \tag{B.3}$$

The approximations are obtained by neglecting the error terms indicated by the O-notation.
These formulas can be derived from a Taylor series expansion around x,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + ... = \sum_{n=0}^{\infty} \frac{h^n}{n!} f^{(n)}(x) \tag{B.4}$$

and

$$f(x+h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) + ... = \sum_{n=0}^{\infty} (-1)^n \frac{h^n}{n!} f^{(n)}(x), \tag{B.5}$$

where $f^{(n)}$ is the n^{th} order derivative of f. Subtracting $f(x)$ from both sides of the above two equations and dividing by h respectively $-h$ leads to he forward difference respectively the backward difference. The central difference is obtained by subtracting equation (B.5) from equation (B.4) and then dividing by $2h$.
The question is how small h has to be in order for the algebraic difference $\frac{f(x+h)-f(x)}{h}$ (for in this case the forward difference approximation) to be good approximation of the derivative. It is clear from the above formulas that the error for the central difference formula is $O(h^2)$. Thus, central differences are significantly better than forward and backward differences.
Higher order derivatives can be approximated using the Taylor series about the value x

$$f(x+2h) = \sum_{n=0}^{\infty} \frac{(2h)^n}{n!} f^{(n)}(x) \tag{B.6}$$

and

$$f(x-2h) = \sum_{n=0}^{\infty} (-1)^n \frac{(2h)^n}{n!} f^{(n)}(x). \tag{B.7}$$

A forward difference approximation to $f''(x)$ is then

$$\frac{f(x+h) - 2f(x+h) + f(x)}{h^2} + O(h), \tag{B.8}$$

and a centered difference approximation is for example

$$\frac{f(x+h) - 2f(x) + f(x+h)}{h^2} + O(h^2). \tag{B.9}$$

Now we discretize the kinetic and potential energy operator. For simplicity, consider the one-dimensional case. We first discretize the interval $[0,1]$ using a uniform grid of N points $x_i = ih, h = \frac{1}{N}, i = 0, 1, ..., N$. It follows that $f(x) \mapsto f(x_i) =: f_i$. The Taylor series expansion of a function about a point x_i becomes

$$f_{i+k} = f_i + \sum_{n=0}^{\infty} (-1)^n \frac{(kh)^n}{n!} f^{(n)}(x), \tag{B.10}$$

where $k = \pm 1, \pm 2, ..., \pm N$. Analogously as above, we can find central difference formulas for f_j', f_j'', namely

$$f_j' = \frac{-f_{j-1} + f_{j+1}}{2h} + O(h^2) \tag{B.11}$$

$$f_j'' = \frac{f_{j-1} - 2f_j + f_{j+1}}{h^2} + O(h^2). \tag{B.12}$$

The approximations are again obtained by neglecting the error terms.
Using this uniform grid with grid spacing $h = 1/N$, it follows that the second derivative operator in one dimension is given by the tridiagonal matrix $\frac{1}{h^2}[\cdots 1 \ -2 \ 1 \cdots]_N$ and the potential which acts as multiplication, is given by a diagonal matrix. With the notation $\frac{1}{h^2}[\cdots 1 \ -2 \ 1 \cdots]_N$, we mean the N-dimensional matrix

$$\frac{1}{h^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}$$

Now suppose that the values of the kinetic energy operator T are non-uniformly dependent of the positions in space. Then one needs to use a non-uniform grid in order to get a good description of the second derivative. We use the central difference approximation and approach f by a Taylor series.
Denote x_j by the j^{th} grid point and $f_k = f(x_k)$. Then the Taylor series of f at x_j can be written as

$$f_k = f_j + \sum_{m=1}^{\infty} \frac{(x_k - x_j)^m}{m!} f_j^{(m)}. \tag{B.13}$$

If we let $h_{j+\frac{1}{2}} = x_{j+1} - x_j$, then similarly as above, for a three-point finite-difference formula i.e., only f_{i+1}, f_i, f_{i-1} are used, we find that

$$f_{j+1} = f_j + h_{j+\frac{1}{2}} f'_j + \frac{h^2_{j+\frac{1}{2}}}{2} f''_j + \frac{h^3_{j+\frac{1}{2}}}{6} f^{(3)}_j + ... \tag{B.14}$$

and similarly for $h_{j-\frac{1}{2}} = x_{j-1} - x_j$, so that $x_j - x_{j-1} = -h_{j-\frac{1}{2}}$, we find

$$f_{j-1} = f_j - h_{j-\frac{1}{2}} f'_j + \frac{h^2_{j-\frac{1}{2}}}{2} f''_j - \frac{h^3_{j-\frac{1}{2}}}{6} f^{(3)}_j + ... \tag{B.15}$$

Both expressions can be used to eliminate f'_j to derive an expression for the second derivative:

$$f''_j = \frac{2f_{j-1}}{h_{j-\frac{1}{2}}(h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}})} - \frac{2f_j}{h_{j-\frac{1}{2}} h_{j+\frac{1}{2}}} + \frac{2f_{j+1}}{h_{j+\frac{1}{2}}(h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}})} + \frac{h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}}}{3} f^{(3)}_j + \mathcal{O}(h^2). \tag{B.16}$$

This is the central difference approximation for the non-uniform grid. If we assume that $h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}}$ is small, we may neglect the last term, and we get precisely that

$$\frac{2}{h_{j-\frac{1}{2}}(h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}})} = T_{j,j-1}, \tag{B.17}$$

$$\frac{-2}{h_{j-\frac{1}{2}} h_{j+\frac{1}{2}}} = T_{j,j}, \tag{B.18}$$

$$\frac{2}{h_{j+\frac{1}{2}}(h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}})} = T_{j,j+1}. \tag{B.19}$$

Therefore we find that the ratio, say ρ_j, equals

$$\rho_j = \frac{T_{j,j+1}}{T_{j,j-1}} = \frac{h_{j-\frac{1}{2}}}{h_{j+\frac{1}{2}}}. \tag{B.20}$$

Thus $h_{j-\frac{1}{2}} = \rho_j h_{j+\frac{1}{2}}$. We derive from this combined with the above three equations that

$$h^2_{j+\frac{1}{2}} = \frac{2}{T_{j,j-1}\rho_j(1+\rho_j)}, \tag{B.21}$$

$$\text{or} \quad h^2_{j+\frac{1}{2}} = \frac{2}{T_{j,j+1}(1+\rho_j)}. \tag{B.22}$$

Appendix C

Semiclassical WKB approximation

In this Appendix, we review some important results of the semiclassical Wentzel-Kramers-Brillouin (WKB) approximation. We give a short overview of the most important results needed for §4.8. The information in this appendix is taken from [34] and [2].

A particle of a mass m satisfies the Schrödinger equation given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = [E - V(x)]\psi. \tag{C.1}$$

This equation is equivalent to

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi, \tag{C.2}$$

where the momentum p is given by

$$p(x) = \begin{cases} \sqrt{2m(E - V(x))}, & E \geqslant V(x) \\ \pm i\sqrt{2m(V(x) - E)}, & E < V(x). \end{cases} \tag{C.3}$$

The generalized de Broglie-wavelength is given by

$$\lambda(x) = \frac{h}{p(x)}, \tag{C.4}$$

where h is the Planck constant. It turns out that there are three cases: the case $E > V(x)$, called the classically *allowed* region; the case $E < V(x)$, called the classically *forbidden* region; and finally the case $E = V(x)$, consisting of turning points.

We start with the first case. In general the wave function ψ has a position x dependent on the phase $\varphi(x)$. It is therefore given by

$$\psi(x) \simeq Ae^{\frac{i}{\hbar}\varphi(x)}, \tag{C.5}$$

with A a normalization constant. Substituting this into (C.1) gives

$$i\hbar\varphi^{(2)} + (\varphi^{(1)})^2 = p^2. \tag{C.6}$$

For $\hbar$ small, we can expand $\varphi(x)$ in terms of $\hbar$, assuming $\varphi(x)$ is a polynomial. We find

$$\varphi(x) = \varphi_0(x) + \hbar\varphi_1(x) + \frac{\hbar^2}{2!}\varphi_2(x) + ... \tag{C.7}$$

Substituting (C.5) into (C.6), and comparing to (C.7) up to the second order, we find the equations:

$$(\varphi_0^{(1)})^2 = p^2, \tag{C.8}$$

$$2\varphi_0^{(1)}\varphi_1^{(1)} - i\varphi_0^{(2)} = 0, \tag{C.9}$$

$$\varphi_0^{(1)}\varphi_1^{(1)} + (\varphi_1^{(1)})^2 + i(\varphi_1^{(2)})^2 = 0. \tag{C.10}$$

Using that $E > V(x)$, so that $p(x)$ is a real, the solution to the first equation is

$$\varphi_0(x) = \pm \int^x p(y)dy, \tag{C.11}$$

where we have a free choice for the lower bound of the integral, since any constant can be absorbed in A. Hence we can solve the second equation:

$$\varphi_1(x) = \frac{i}{2}\log(p(x)). \tag{C.12}$$

The solution to the third equation is then given by

$$\varphi_2(x) = \mp\frac{p'(x)}{2p^2(x)} \mp \int^x p(y)\left(\frac{p'(y)}{2p^2(y)}\right)^2 dy. \tag{C.13}$$

If $|\hbar\varphi_2(x)/2 << 1|$, then the power series (C.7) can be terminated after two terms. This can only hold if

$$\left|\frac{p'(x)}{2p^2(x)}\right| << \frac{2}{\hbar}. \tag{C.14}$$

This is the case when to potential $V(x)$ varies slowly as a function of position, or when $\hbar \to 0$.
If we assume (C.14), then we may truncate the power series after two terms. Plugging in our solution for φ_0 and φ_1, we find the *WKB approximation* for the wave function:

$$\frac{A}{\sqrt{p(x)}} e^{\pm\frac{i}{\hbar}\int^x p(y)dy}. \tag{C.15}$$

The general solution under these semiclassical assumptions is

$$\psi(x) \simeq \frac{1}{\sqrt{p(x)}}\left(Ae^{\frac{i}{\hbar}\int^x p(y)dy} + Be^{-\frac{i}{\hbar}\int^x p(y)dy}\right). \tag{C.16}$$

For the second case, the classical forbidden region, we have $E < V(x)$, so that $p(x)$ is imaginary. Similarly as above, one can deduce that the general solution of the wave function (under this assumption (C.14)) is

$$\psi(x) \simeq \frac{1}{\sqrt{p(x)}}\left(Ce^{\frac{1}{\hbar}\int^x |p(y)|dy} + De^{-\frac{1}{\hbar}\int^x |p(y)|dy}\right). \tag{C.17}$$

As we have argued, the approximations to the wave functions for the two previous cases, only make sense if (C.14) holds. However, close to the classical turning points, we see that $p(x)$ approximates zero. Therefore, there is some area where (C.14) is not valid, and hence the WKB approximation derived above is not applicable there. First, we should remark there are two kinds of turning points. In the figure below, x_1 is a left-hand turning point and x_2 is a right-hand turning point.

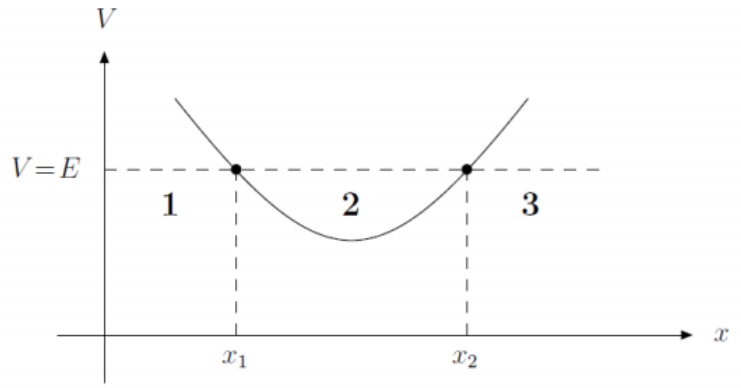

Figure C.1: A general potential well. The particle has energy E. The turning points are indicated by x_1 and x_2, the three different areas by 1, 2 and 3. This picture has been taken from [2].

In order to find the WKB wave functions around these turning points, one needs to use a different approach. We won't derive these functions but refer to [34]. The wave function around the right-hand turning point is given by

$$\psi(x) \simeq \begin{cases} \frac{1}{\sqrt{p(x)}}\left[2C\cos\left(\frac{1}{\hbar}\int_{x_2}^{x}|p(y)|dy+\frac{\pi}{4}\right)+D\sin\left(\frac{1}{\hbar}\int_{x_2}^{x}|p(y)|dy+\frac{\pi}{4}\right)\right], & \text{if } x\leqslant x_2 \\ \frac{1}{\sqrt{|p(x)|}}\left[C\exp-\frac{1}{\hbar}\int_{x_2}^{x}|p(y)|dy+D\exp-\frac{1}{\hbar}\int_{x}^{x_2}|p(y)|dy\right], & \text{if } x>x_2, \end{cases} \tag{C.18}$$

A similar result holds for the left-hand turning point.

Appendix D

Schrödinger operators

We provide the preliminaries for the theory of unbounded operators, as used in §5.4. We just state some definitions and basic facts. In particular, we introduce the term Schrödinger operator. This appendix is based on [31] and [32].

Definition D.1. *Let T be a mapping from a Hilbert space $\mathcal{H}_1$ into a Hilbert space $\mathcal{H}_2$. The graph of T, denoted by $\Gamma(T)$, is defined as*

$$\Gamma(T) = \{(x, y) \mid \ (x, y) \in \mathcal{H}_1 \times \mathcal{H}_2, \ y = Tx\}. \tag{D.1}$$

The graph of T is thus a linear subset of $\mathcal{H}_1 \times \mathcal{H}_2$, which is a Hilbert space $\mathcal{H}_1 \oplus \mathcal{H}_2$ with inner product

$$\langle(\psi_1, \varphi_1), (\psi_2, \varphi_2)\rangle = \langle\psi_1, \psi_2\rangle + \langle\varphi_1, \varphi_2\rangle. \tag{D.2}$$

Definition D.2. *An operator $T : \mathcal{H}_1 \to \mathcal{H}_2$ is said to be closed if the graph $\Gamma(T)$ is a closed subset of $\mathcal{H}_1 \times \mathcal{H}_2$.*

Definition D.3. *Let T_1 and T be operators on $\mathcal{H}$. if $\Gamma(T_1) \supset \Gamma(T)$, then T_1 is said to be an extension of T, and we write $T_1 \supset T$. Equivalently, $T_1 \supset T$ if and only if $D(T_1) \supset D(T)$, and $T_1(\varphi) = T(\varphi)$ for all $\varphi \in D(T)$. Here, $D(T)$ is called the domain of T.*

Definition D.4. *An operator T is closable if it has a closed extension. Every closable operator has a smallest closed extension, called its closure, which we denote by $\overline{T}$.*

Definition D.5. *The domain of an operator T on a Hilbert space $\mathcal{H}$ is a linear subspace $\mathcal{H}$, denoted by $D(T)$. If the domain is dense in $\mathcal{H}$, we say that T is densely defined. Unless specified otherwise, we will always suppose that the domain is dense.*

Definition D.6. *An unbounded linear operator T from $\mathcal{H}_1$ to $\mathcal{H}_2$ is a pair $(D(T), T)$ consisting of a domain $D(T) \subset \mathcal{H}_1$ and a linear map $T : D(T) \subset \mathcal{H}_1 \to \mathcal{H}_2$.*

Remark : unbounded operators may be bounded according to our terminology.

Definition D.7. *Let T be a densily defined operator on a Hilbert space $\mathcal{H}$. Let $D(T^*)$ be the set of $\varphi \in \mathcal{H}$ for which there is a $\eta \in \mathcal{H}$ with*

$$\langle T\psi, \varphi\rangle = \langle\psi, \eta\rangle, \quad \text{for all } \ \psi \in D(T). \tag{D.3}$$

For each such $\varphi \in D(T^*)$, we define $T^*(\varphi) = \eta$. T^* is called the adjoint of T. By the Riesz Lemma, $\varphi \in D(T^*)$ if and only if $|\langle T\psi, \varphi\rangle| \leqslant C||\psi||$, for all $\psi \in D(T)$.

Definition D.8. *Let T be a closed operator on a Hilbert space $\mathcal{H}$. A complex number λ is in the resolvent set $\rho(T)$ if $\lambda I - T$ is a bijection of $D(T)$ onto $\mathcal{H}$ with a bounded inverse. If $\lambda \in \rho(T), R_\lambda(T) = (\lambda I - T)^{-1}$ is called the resolvent of T at λ.*

Definition D.9. *A densely defined operator T on a Hilbert space is called symmetric (or Hermitian) if $T \subset T^*$, that is $D(T) \subset D(T^*)$ and $T\varphi = T^*\varphi$ for all $\varphi \in D(T)$. Equivalently, T is symmetric if and only if*

$$\langle T\varphi, \psi\rangle = \langle \varphi, T\psi\rangle, \quad \text{for all } \ \varphi, \psi \in D(T). \tag{D.4}$$

Definition D.10. *T is called self-adjoint if $T = T^*$, that is if and only if T is symmetric and $D(T) = D(T^*)$.*

A symmetric operator is always closable since $D(T^*) \supset D(T)$ is dense in $\mathcal{H}$. If T is symmetric, T^* is a closed extension of T, so the smallest closed extension T^{**} of T must be contained in T. Thus for symmetric operators we have $T \subset T^{**} \subset T^*$. For closed symmetric operators, we have $T = T^{**} \subset T^*$, and for self-adjoint operators we have $T = T^{**} = T^*$.
From this, one can easily see that a closed symmetric operator T is self-adjoint if and only if T^* is symmetric.

Definition D.11. *A symmetric operator T is called essentially self-adjoint if its closure $\bar{T}$ is self-adjoint. If T is closed, a subset $D \subset D(T)$ is called a core for T if $T\restriction_D = T$.*

One can show that if T is essentially self-adjoint, then it has only one self-adjoint extension, namely its closure. The converse is also true.

Definition D.12. *A densely defined symmetric operator T, on a domain $D(T)$ is called positive if*

$$\langle T\psi, \psi\rangle \geqslant 0 \quad (\psi \in D(T)). \tag{D.5}$$

The following theorem will be useful when proving properties of the closure operator.

Theorem D.13 (Friedrichs)**.** *A positive, densely defined, symmetric operator a, has a unqiue positive self-adjoint extension, called the Friedrichs extension. When a is essentially self-adjoint, this extension (of course) equals the closure of a.*

Definition D.14. *A quadratic form is a map $q : Q(Q) \times Q(q) \to \mathbb{C}$, where $Q(q)$ is a dense linear subset of $\mathcal{H}$ called the form domain, such that $Q(\dot{;}\psi)$ is conjugate linear and $Q(\varphi, \dot{)}$ is linear for $\varphi, \psi \in Q(q)$. If $Q(\varphi, \psi) = Q(\bar{\psi}, \varphi)$, we say hat q is symmetric. If $q(\varphi, \varphi) \geqslant 0$, for all $\varphi \in Q$, q is called positive, and if $q(\varphi, \varphi) \geqslant -M||\varphi||^2$, for some M, we say q is semibounded.*

Definition D.15. *A Schrödinger operator is a self-adjoint operator H on a dense domain $D(H)$ of the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$, such that H can be written as the sum of the minus the Laplace-operator (Laplacian) and multiplication with a given real function V, also called the potential. Thus V is seen as the (pointwise) multiplication operator with V.*
A priori, the function V is not continuous or bounded, but it needs to be at least locally integrable.

An example of a Schrödinger operator in one dimension is the operator $\tilde{h}_2$ given by (4.72).

Definition D.16. *An operator $T : D(T) \subset \mathcal{H}_1 \to \mathcal{H}_2$ has compact resolvent at λ if $R_\lambda(T)$ is a compact operator, i.e., the closure of $R_\lambda(T)(B)$ is a compact subset of $\mathcal{H}_2$, where B is the closed unit ball. .*

Definition D.17. *Let T_n be self-adjoint operators, $n = 1, 2, ...$ Then T_n is said to converge to T in the norm resolvent sense if $R_\lambda(T_n) \to R_{\lambda(T)}$ in norm for all λ with $Im(\lambda) \neq 0$. T_n is said to converge to T in the strong resolvent sense if $R_\lambda(T_n) \to R_\lambda(T)$ strongly for all λ with $Im(\lambda) \neq 0$.*

Remark.
It can be shown in [31, Thm. VIII.19] that for a sequence A_n of self-adjoint operators and for a point $\lambda_0 \in \mathbb{C}$, if $\mathrm{Im}(\lambda_0) \neq 0$ and $R_{\lambda_0}(A_n)\varphi \to R_{\lambda_0}(A)\varphi$ for all $\varphi \in \mathcal{H}$, then $A_n \to A$ is the strong resolvent sense.

In order to prove some theorems in §5.4, we need the notion of a Sobolev space, see also [9].

Definition D.18. *Let Ω be an open subset of $\mathbb{R}^n$. Let $k \in \mathbb{N}$ and $p \in [1, \infty]$. The Sobolev space $W^{k,p}(\Omega)$ is defined to be the set of all functions f on Ω such that for every multi-index α, with $|\alpha| \leqslant k$, the mixed partial derivative*

$$f^{(\alpha)} = \frac{\partial^{|\alpha|} f}{\partial_{x_1}^{\alpha_1} \cdots \partial_{x_n}^{\alpha_n}}, \tag{D.6}$$

exists in the weak sense and is in $L^p(\Omega)$, i.e., $||f^{(\alpha)}||_{L^p} < \infty$. That is, the Sobolev space $W^{k,p}(\Omega)$ is defined as

$$W^{k,p}(\Omega) = \{u \in L^p(\Omega) \mid \ D^\alpha u \in L^p(\Omega), \ \forall \ |\alpha| \leqslant k\}. \tag{D.7}$$

For $p = 2$, we use the notation $H^k = W^{k,2}$. It can be shown that H^k is a Hilbert space for all $k \in \mathbb{N}$ with inner product

$$\langle u, v \rangle_{H^k} = \sum_{|a| \leqslant k} \langle D^\alpha u, D^\alpha v \rangle_{L^2}. \tag{D.8}$$

There exists also Sobolev space spaces with non-negative real parameter. Assume $0 < s < \infty$ and $u \in L^2(\mathbb{R}^n)$. Then, we define the space $H^s(\mathbb{R}^n)$ by

$$H^s(\mathbb{R}^n) = \{u \in L^2(\mathbb{R}^n) | \ (1 + |y|^s)\hat{u} \in L^2(\mathbb{R}^n)\}, \tag{D.9}$$

where we denote the Fourier transform of any $u \in L^2(\mathbb{R}^n)$ by $\hat{u}$. For non-negative integer s, we make $H^s(\mathbb{R}^n)$ into a Hilbert space with norm

$$||u||_{H^s} = ||(1 + |y|^s)\hat{u}||_{L^2}. \tag{D.10}$$

The spaces $H^s(L^2(\mathbb{R}^n))$ are called fractional Sobolev spaces.

The next theorem describes when the domain of the Schrödinger operator is bounded. It can be found in [12, p.43]

Theorem D.19. *Let Λ be a cube in $\mathbb{R}^d$, and V a continuous function on Λ. Then the Schrodinger operator $H = -\Delta + V$, acting on the space $L^2(\Lambda)$ with Dirichlet boundary conditions, has purely point spectrum, accumulating at ∞.*

Appendix E

Deformation quantization

In this appendix we will give the basics of the notion of a continuous bundle of C^*-algebras and a deformation quantization, including an example. A rigorous treatment can be found in [22, Def. C.121], [22, Def. 7.1], and [22, pp. 250-252]. The main results of this appendix have been used in chapter 6.

Definition E.1. *Let I be a locally compact Hausdorff space. A continuous bundle of C^*-algebras over I consists of a C^*-algebra A, a collection of C^*-algebras $(A_\hbar)_{\hbar\in I}$ with norms $||\cdot||_\hbar$, and surjective homomorphisms $\varphi_\hbar : A \to A_\hbar$ for each $\hbar \in I$, such that:*

1. The function $\hbar \mapsto ||\varphi_\hbar(a)||_\hbar$ is in $C_0(I)$ for all $a \in A$.

2.The norm for any $a \in A$ is given by

$$||a|| = sup_{\hbar\in I}||\varphi_\hbar(a)||_\hbar. \tag{E.1}$$

3. For any $f \in C_0(I)$ and $a \in A$, there is an element $fa \in A$ such that for each $\hbar \in I$,

$$\varphi_\hbar(fa) = f(\hbar)\varphi_\hbar(a). \tag{E.2}$$

A continuous (cross-) section of the bundle in question is a map $\hbar \mapsto a(\hbar) \in A_\hbar$, $(\hbar \in I)$, for which there exists an $a \in A$ such that $a(\hbar) = \varphi_\hbar(a)$ for each $\hbar \in I$.

For the definition below, we will assume that the space I is taken to be a subset of the unit interval $[0, 1]$ that contains 0 as an accumulation point (so one may have for example $I = [0, 1]$ itself, or $I = (1/\mathbb{N}) \cup \{0\}$).

Definition E.2. *A deformation quantization of a Poisson manifold X consists of a continuous bundle of C^*-algebras $(A, \{\varphi : A \to A_\hbar\}_{\hbar\in I})$ over I, along with maps*

$$Q_\hbar : \tilde{A}_0 \to A_\hbar \quad (\hbar \in I), \tag{E.3}$$

where $\tilde{A}_0$ is a dense subspace of $A_0 = C_0(X)$, such that:

1. Q_0 is the inclusion map $\tilde{A}_0 \hookrightarrow A_0$;

2. Each map $Q_\hbar$ is linear and satisfies $Q_\hbar(f^*) = Q_\hbar(f)^*$.

3. For each $f \in \tilde{A}_0$, the following map is a continuous section of the bundle:

$$0 \to f \tag{E.4}$$

$$\hbar \to Q_\hbar(f) \quad (\hbar > 0) \tag{E.5}$$

4. For all $f, g \in \tilde{A}_0$ one has the Dirac-Groenewold-Rieffel condition:

$$\lim_{\hbar\to 0} ||\frac{i}{\hbar}[Q_\hbar(f), Q_\hbar(g)] - Q_\hbar(\{f,g\})||_\hbar = 0. \tag{E.6}$$

it follows from the definitions of a continuous bundle that continuity properties like

$$\lim_{\hbar\to 0} ||Q_\hbar(f)|| = ||f||_\infty; \tag{E.7}$$

$$\lim_{\hbar\to 0} ||Q_\hbar(f)Q_\hbar(g) - Q_\hbar(fg)|| = 0, \tag{E.8}$$

are automatically satisfied. if X is compact, so that $1_X \in C_0(X)$, and we require $Q_\hbar(1_X) = 1_H$, with 1_H the unit of the C^*-algebra $A_\hbar$.

We give an example without proof for the case $n = 1$. We put

$$A_0 = C_0(T^*(\mathbb{R})); \tag{E.9}$$

$$A_\hbar = B_0(L^2(\mathbb{R})), \quad (\hbar > 0), \tag{E.10}$$

where we identity the cotangent bundle $T^*(\mathbb{R}) \simeq \mathbb{R}^2$, carries the canonical Poisson structure given by

$$\{f,g\} = \sum_{j=1}^{2} \left(\frac{\partial f}{\partial p_j}\frac{\partial g}{\partial q^j} - \frac{\partial f}{\partial q^j}\frac{\partial g}{\partial p_j} \right), \tag{E.11}$$

where $(p,q) \in \mathbb{R}^2$ The C^*-algebra $A_\hbar$ is the space of compact operators on the Hilbert space $L^2(\mathbb{R})$. A deformation quantization of $\mathbb{R}^2$ that is *positive* in the sense that

$$f \geqslant 0 \implies Q_\hbar(f) \geqslant 0, \quad (f \in \tilde{A}_0 \subset A_0) \tag{E.12}$$

exists under the name Berezin quantization, denoted by $Q^B_\hbar$. For this we need the notation of a coherent state. For each $(p,q) \in \mathbb{R}^2$, and $\hbar > 0$, define a unit vector $\phi^{(p,q)}_\hbar \in L^2(\mathbb{R})$ by

$$\phi^{(p,q)}_\hbar(x) = (\pi\hbar)^{-n/4} e^{-ipq/2\hbar} e^{ipx/\hbar} e^{-(x-q)^2/2\hbar}. \tag{E.13}$$

This is called a coherent state. Writing $z = p + iq$, the transition probability between two coherent states is

$$|\langle \phi^{(z)}_\hbar, \phi^{(z')}_\hbar \rangle|^2 = e^{-|z-z'|^2/2\hbar}. \tag{E.14}$$

Then we define $Q^B_\hbar : C_0(T^*\mathbb{R}) \to B_0(L^2(\mathbb{R}))$, by

$$Q^B_\hbar(f) = \int_{\mathbb{R}^2} \frac{dpdq}{2\pi\hbar} f(p,q) |\phi^{(p,q)}_\hbar\rangle\langle\phi^{(p,q)}_\hbar|. \tag{E.15}$$

The integral is understood in the sense that for $\psi, \varphi \in L^2(\mathbb{R})$, we have

$$\omega_\psi(Q^B_\hbar(f)) := \langle \varphi, Q^B_\hbar(f)\psi\rangle = \int_{\mathbb{R}^2} \frac{dpdq}{2\pi\hbar} f(p,q) \langle \varphi, \phi^{(p,q)}_\hbar\rangle\langle\phi^{(p,q)}_\hbar, \psi\rangle. \tag{E.16}$$

In particular, for each unit vector ψ we may write

$$\langle \psi, Q^B_\hbar(f)\psi\rangle = \int_{\mathbb{R}^2} d\mu_\psi f, \tag{E.17}$$

where μ_ψ is the probability measure on $T^*(\mathbb{R})$ with density

$$B_\hbar^\psi(p,q) = |\langle \phi_\hbar^{(p,q)}, \psi\rangle|^2, \tag{E.18}$$

called the Husimi function of $\psi \in L^2(\mathbb{R})$; in other words, μ_ψ is given by

$$d\mu_\psi = \frac{dpdq}{2\pi\hbar} B_\hbar^\psi(p,q). \tag{E.19}$$

In general, ψ depends on $\hbar$ as it corresponds to a $\hbar$-dependent Schrödinger operator. For example, $\psi_\hbar$ can be the ground state eigenfunction. We say that the wave-functions $\psi_\hbar$ have a classical limit if

$$\lim_{\hbar\to 0} \int_{T\mathbb{R}^2} d\mu_{\psi_\hbar} f = \int_{\mathbb{R}^2} d\mu_0 f, \tag{E.20}$$

for any $f \in C_0(T^*(\mathbb{R}))$, where μ_0 is some probability measure on $T^*(\mathbb{R}) \cong \mathbb{R}^2$.

In the remaining part of this appendix, we introduce the notion of (quasi) symmetric sequences and show how they play a role in continuous bundles of C^*-algebras. For this, we first explain how to link an element of B^M to an element of B^N, with B^N the N-fold tensor product of B, and B a unital C^*-algebra describing a single quantum spin system. The case $B = M_2(\mathbb{C})$ will be used in this thesis. We define $\mathcal{S}_N$ to be the permutation group of N objects acting on B^N in the obvious way, i.e., by linear and continuous extension of

$$\alpha_p^{(N)}(b_1 \otimes \cdots \otimes b_N) = b_{p(1)} \otimes \cdots \otimes b_{p(N)}, \tag{E.21}$$

where $B_i \in B$, and $p \in \mathcal{S}_N$. This yields a Symmetrizer operator $S_N : B^N \to B^N$, defined by

$$S_N = \frac{1}{N!} \sum_{p\in\mathcal{S}_N} \alpha_p^{(N)}. \tag{E.22}$$

It can be shown that S^N is continuous. For $N \geqslant M$, we then define

$$S_{M,N} : B^M \to B^N \tag{E.23}$$

by linear (and if necessary continuous) extension of

$$S_{M,N}(a_{1/M}) = S_N(a_{1/M} \otimes \mathbf{1}_B \cdots \mathbf{1}_B) \quad (a_{1/M} \in B^M), \tag{E.24}$$

with $N - M$ copies of the unit $\mathbf{1}_B \in B$,so as to obtain an element of B^N. Clearly, $S_{N,N} = S_N$. In particular $S_{1,N} : B \to B^N$ gives the average of b over N copies of B:

$$S_{1,N}(b) = \frac{1}{N} \sum_{k=1}^{N} \mathbf{1}_B \otimes \cdots b_{(k)} \otimes \mathbf{1}_B \cdots \otimes \mathbf{1}_B. \tag{E.25}$$

Finally, we give the definition of symmetric and quasi-symmetric sequences. They play a role in the continuous bundle of C^*-algebras $A_0^{(c)} = C(S(B))$ and $A_{1/N}^{(c)} = B^N$, with B^N the N-fold tensor product of the unital C^*-algebra B.

Definition E.3. *We say that a sequence $(a_{1/N})_{N\in\mathbb{N}}$, with $a_{1/N} \in B^N$ is symmetric, when there exists an $M \in \mathbb{N}$ and $a_{1/M} \in B^M$ such that for each $N \geqslant M$ one has*

$$a_{1/N} = S_{M,N}(a_{1/N}). \tag{E.26}$$

This implies that $a_{1/M} = S_M(a_{1/M})$. For each symmetric sequence we define a function $a_0 : S(B) \to \mathbb{C}$ by

$$a_0(\omega) = \lim_{n\to\infty} \omega^N(a_{1/N}), \tag{E.27}$$

where $\omega \in S(B)$, and $\omega^N \in S(B^N)$ is defined by a linear and coninuous extension of

$$\omega^N(b_1 \otimes \cdots \otimes b_N) = \omega(b_1) \otimes \cdots \omega(b_N). \tag{E.28}$$

Continuity of ω^N is guaranteed by [22, C.98]. It can be shown, using the fact that the sequence is symmetric, that the above limit exists from which it follows that $a_0 \in C(S(B))$.

We now return to the general case.

Definition E.4. *A sequence $(a_{1/N})_{N\in\mathbb{N}}$ as above is $\underline{quasi-symmetric}$ if for each $N \in \mathbb{N}$ one has $a_{1/N} = S_N(a_{1/N})$ and for any $\epsilon > 0$ there is a symmetric sequence $(\tilde{a}_{1/N})$ and some $M \in \mathbb{N}$ such that $||a_{1/N} - \tilde{a}_{1/N}|| < \epsilon$ for all $N > M$.*

This brings us to an important theorem.

Theorem E.5. *For any unital C^*-algebra B, the C^*-algebras*

$$A_0^{(c)} = C(S(B)); \tag{E.29}$$

$$A_{1/N}^{(c)} = B^N, \tag{E.30}$$

where B^N is the N-fold projective tensor power $\hat{\bigotimes}_{max}^N B$, are the fibers of a continuous bundle $A^{(c)}$ of C^*-algebras over $I = (1/\mathbb{N}) \cup \{0\}$ whose continuous cross-sections are the quasi-symmetric sequences $(a_{1/N})$ with limit a_0 given by (E.27).

The proof is very technical and will be omitted (See e.g. [22, Thm. 8.4]). In any case, it can be shown that we have deformation quantization of $S(B)$ in the sense of (E.2) [22, Thm. 8.4].

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